Second Variations of the Causal Action for Regularized Dirac Sea Configurations

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Summary

The theory of causal fermion systems provides a new mathematical framework which allows for a unified description of contemporary fundamental physics. One essential ingredient of this framework is the so-called *causal action* which is a certain functional of a measure defined on a specific subset of the bounded linear operators on a Hilbert space. For a given measure, this functional can be regarded as a quantifier of the weighted causal relation of all operators within the support of the measure. Moreover, the functional is subject to the *causal action principle* which aims at minimizing the causal action by varying the measure and in this way makes the measure a dynamical variable. All of this, as well as further fundamental objects of the theory which are relevant to this thesis, are introduced and explained in Chapter 1.

Within these structures and based on certain foundational conceptions, one can now model concrete physical systems, which are always understood as a combination of some spacetime manifold together with the fermionic particle content existing therein. The foundational conception underlying the modelling is to regard fermions as the fundamental building blocks of nature and to conceive the vacuum, according to Dirac's interpretation, as the presence of all negative-energy solutions of the Dirac equation in the respective spacetime. To get into the framework of the theory of causal fermion systems, one chooses the above-mentioned Hilbert space as these negative-energy solutions and simultaneously forgets about all the other geometrical and topological structures of spacetime. In order to take into account a possibly existing, though yet not observed, non-trivial microstructure of spacetime which leads to a modified high-energy behaviour of the Dirac solutions, the elements of the Hilbert space are equipped with a so-called *regularization*. As will be explained in further detail in Chapter 2, it is this regularization which in the modelling of a physical system within the structures provided by the theory of causal fermion systems plays the role of the measure and is thus dynamically determined through the causal action principle.

Embedded in this setting, the present thesis is concerned with the derivation and analysis of the multipole expansion of second variations of the above-mentioned causal action which are caused by variations of the regularization of the so-called *regularized kernel of the fermionic projector*. The thesis is divided into three major parts: In Part I: Basics we lay the foundations by first introducing and discussing the fundamental mathematical structures of the theory of causal fermion systems and subsequently explaining in detail how concrete physical systems can be realized within this abstract setting and what exactly the underlying foundational conceptions are. Part II: Developments is devoted to the derivation of the multipole expansion of second variations of the *regularized causal action*. More specifically, in Chapter 3 we derive second variations of the regularized causal action for a homogeneous regularized kernel of the fermionic projector having vector-scalar structure which results in Theorem 3.4.3. Starting from this result, the multipole expansion of the second variation of the regularized causal action is derived and simplified through several steps in Chapter 4, ultimately leading to Theorem 4.3.1 which expresses the multipole moments of the second variation of the regularized causal action in terms of integral operators. In Part III: Applications we then analyze the second variation of the regularized causal action for special regularizations. More concretely, in Chapter 5 we consider an anisotropic generalization of the so-called iε*-regularization* which is extensively studied in the literature and demonstrate in Theorem 5.2.5 that Lorentz boosts of the velocity vector of this regularization leave the regularized causal action invariant. Additionally, we prove that *anisotropically* iε*-regularized kernels of the fermionic projector* lead to a non-vanishing second-order variation of the local particle density compared with the symmetric situation. Finally, in Chapter 6 we outline a procedure which, under certain simplifying assumptions, ultimately allows to demonstrate invertibility of the lowest-order multipole moment of the second variation of the regularized causal action. A generalization of this approach to higher multipole moments is part of a novel mechanism of baryogenesis within the theory of causal fermion systems.

To Marina, the love of my life

Acknowledgement

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Within the academic ecosystem, I furthermore want to thank my office colleague Dr. Andreas Platzer for sharing his knowledge on causal fermion systems by willingly answering numerous questions, especially during the first months in Regensburg, and in this way facilitating the process of familiarization with the whole theory. Likewise, I want to thank my office colleague Saeed Zafari for helpful discussions and, in particular, for encouraging conversations in times of stagnation which probably befall every doctoral student sooner or later. Also, I am greatly indebted to Dr. Marco Oppio, who not only had a sympathetic ear for questions on technical details at any time, but who also was a great personal asset to our entire working group. A heartfelt *"Thank You"* to the three of you for the wonderful time and, of course, for our regular *pause caffè*. Special thanks goes to Dr. Claudio Paganini for inviting me to a research stay at Monash University in Melbourne. Whenever I think back to those weeks which left a lasting impression, I feel deep gratitude for the warm welcome and kind hospitality on the other side of the earth. I very much enjoyed every single minute of this time with all the inspiring, insightful and sometimes almost philosophical discussions on the foundations of the theory of causal fermion systems. To counterbalance the daily scientific work, I very much enjoyed being part of the University's Symphonic Wind Orchestra as a clarinetist and for having the honor to serve as its principal conductor for two terms. I will not forget the moments of great musical and emotional intensity created by the many excellent and dedicated musicians I had the chance to meet during this time.

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Finally, I want to send heartfelt thanks to two special persons: First, to my mentor and dear friend Dr. Markus Lackermair who for more than half of my life not only had a decisive influence on my development, but who has shaped both my thinking and my whole being more than anyone else. And, of course, to Marina, who with her unconditional love, her sunshine personality and reliable support both in lighthearted, but especially in dark times has ensured that worries and doubts do not gain the upper hand.

Notation and Conventions

Color Legend

Definitions and definition-like environments such as notations, terminology, and conventions are highlighted by a bar from the green color spectrum. Gray bars indicate lemmas and propositions, while auxiliary calculations (which exclusively occur in the appendices) remain without any color highlighting. Finally, theorems and remarks are highlighted by dark red bars and dark gray bars, respectively.

Number Systems

For the natural numbers we use the convention $\mathbb{N} := \{1, 2, 3, \dots\}$ and denote the natural numbers with zero included by $\mathbb{N}_0$. Likewise, for the positive real numbers we write $\mathbb{R}^+$ and denote the case with zero included by $\mathbb{R}^+_0$.

Matrices

For an n-component vector $v \in \mathbb{K}^n$ with $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ we denote by D_v the associated $n \times n$ diagonal matrix with entries $(D_v)_{ii} = v_i$. Furthermore, by $\mathbb{1}_{m\times n}$ we denote the $(m \times n)$-matrix of ones. Similarly, the $(m \times n)$-matrix of zeroes is denoted by $\mathbf{0}_{m\times n}$. For $n \times n$ square matrices, we write $\mathbb{1}_n := \mathbb{1}_{n\times n}$ and $\mathbf{0}_n := \mathbf{0}_{m\times n}$.

Elements of the Operator Set $\mathcal{F}_n$ and of Physical Spacetime $\mathscr{M}$

To distinguish between elements of the operator set $\mathcal{F}_n$ and elements of physical spacetime $\mathscr{M}$, we consistently use different fonts $x, y, z \in \mathcal{F}_n$ in contrast with $\mathcal{x}, \mathcal{y}, \mathcal{z} \in \mathscr{M}$.[1] Moreover, unless otherwise specified, $(\mathscr{M}, g)$ denotes an m-dimensional semi-Riemannian manifold with signature $(+1, -1, -1, \dots, -1)$.

Indices and Einstein Summation Convention

Concerning indices of four-vectors, we adopt Finster's convention[2] according to which Latin indices denote the components of four-vectors while Greek indices are reserved exclusively for spatial components. This is just the opposite of the convention commonly used in physics.[3, 4] We employ the Einstein summation convention with the addition that for purely spatial indices (indicated by Greek letters) also two upper or two lower indices trigger a summation over the spatial index set.

Multipole Indices

Multipole indices are denoted by (l, m) and (l', m'). Furthermore, for summations over multipole indices we often use the abbreviating notation

$$\sum_{l,m} := \sum_{l=0}^{\infty} \sum_{m=-l}^{l}$$

Regularization and Regularization Length

The superscript $(\,\cdot\,)^\varepsilon$ indicates regularized objects which includes both the type of regularization as well as the regularization length. When talking about ε alone, the regularization length is meant.

Sesquilinear Form

For sesquilinear forms $s : V \times V \to \mathbb{C}$ on complex vector spaces V, we adopt the *physics convention* according to which s is conjugate-linear in the first argument and linear in the second argument.

[1] We remark that this convention was introduced by Finster and Kleiner.[1, Sec. 2]

[2] Note that this is the convention used by Hawking and Ellis.[2, Ch. 4, p. 82] For a listing of the different index and sign conventions, we refer to the corresponding table by Misner, Thorne and Wheeler.[3]

Part I

Basics

Introduction to the Theory of Causal Fermion Systems

1

The Fundamental Mathematical Structures of the Theory of Causal Fermion Systems

Contents

The theory of causal fermion systems provides a rich framework of mathematical objects, structures and mechanisms which together allow for a novel description of fundamental physics in a unified way. The development of the theory of causal fermion systems by Felix Finster over the past two decades has not only produced a steadily growing number of new objects and structures, but also led to a gradual evolution regarding the presentation of the whole framework without changing its conceptual core: While in the early days of the theory[5],[6] the emphasis was on the so-called *fermionic projector* together with the associated *principle of the fermionic projector*, the reformulation of the variational principle in terms of measures on certain Borel sets of finite-rank linear operators on Hilbert spaces[7] marks the beginning[8],[9] of the transition[1] to today's presentation in which the fermionic projector still plays the central role, but in a more general setting which starts from the notion of *causal fermion systems*.[11] In order to have a solid basis for all further chapters, we summarize the fundamental mathematical structures of the theory in its "modern" formulation in Sections 1.1 to 1.3, before in Section 1.4 further structures which are of particular importance for concrete calculations, are reviewed.

[1]The transition from the earlier to the current formulation occurred during Daniela Schiefeneder's doctoral studies and has accordingly found its reflection in chapter 2 of her doctoral thesis.[10, Ch. 2]

1.1 Causal Fermion Systems

The central and eponymous object of investigation in the theory of causal fermion systems are so-called *causal fermion systems* which are a specific composition of mathematical structures.[11, Def. 1.1.1]

Definition 1.1.1 (Causal Fermion System)

A *causal fermion system of spin dimension n* is an ordered triple $(\mathcal{H}_\mathbb{C}, \mathcal{F}_n, \rho)$ consisting of the following structures:

(1) $\mathcal{H}_\mathbb{C}$ denotes a separable, complex Hilbert space $(\mathcal{H}_\mathbb{C}, \langle\cdot|\cdot\rangle_{\mathcal{H}_\mathbb{C}})$

(2) $\mathcal{F}_n$ denotes the subset $\mathcal{F}_n \subset \mathrm{L}(\mathcal{H}_\mathbb{C}, \mathcal{H}_\mathbb{C})$ of self-adjoint, finite-rank, bounded linear operators on $\mathcal{H}_\mathbb{C}$, which – counting multiplicities – have at most $n \in \mathbb{N}$ positive and at most $n \in \mathbb{N}$ negative eigenvalues

(3) ρ denotes a positive measure $\rho : \mathcal{B}(\mathcal{F}_n) \to \mathbb{R}_0^+ \cup \{\infty\}$ on the measurable space $(\mathcal{F}_n, \mathcal{B}(\mathcal{F}_n))$ and is referred to as *universal measure* where

   (a) $\mathcal{T}_{\|\cdot\|}$ denotes the topology induced by the operator norm $\|\cdot\|_{\mathrm{L}(\mathcal{H}_\mathbb{C},\mathcal{H}_\mathbb{C})}$ on $\mathrm{L}(\mathcal{H}_\mathbb{C}, \mathcal{H}_\mathbb{C})$[a]

   (b) $\mathcal{B}(\mathcal{F}_n)$ denotes the Borel-σ-algebra on the topological space $(\mathcal{F}_n, \mathcal{T}_{\mathcal{F}_n})$ where $\mathcal{T}_{\mathcal{F}_n}$ is the subspace topology on $\mathcal{F}_n$ with respect to the topological space $(\mathrm{L}(\mathcal{H}_\mathbb{C}, \mathcal{H}_\mathbb{C}), \mathcal{T}_{\|\cdot\|})$

[a] The operator norm $\|\cdot\|_{\mathrm{L}(\mathcal{H}_\mathbb{C},\mathcal{H}_\mathbb{C})}$ is defined as $\|x\|_{\mathrm{L}(\mathcal{H}_\mathbb{C},\mathcal{H}_\mathbb{C})} := \sup_{u\in\mathcal{H}_\mathbb{C}}\{\|xu\|_{\mathcal{H}_\mathbb{C}} \mid \|u\|_{\mathcal{H}_\mathbb{C}} = 1\}$

Analyzing this definition, one recognizes that a causal fermion system may be regarded as a three-layer system of structures as depicted in Figure 1.1: Based on an underlying Hilbert space

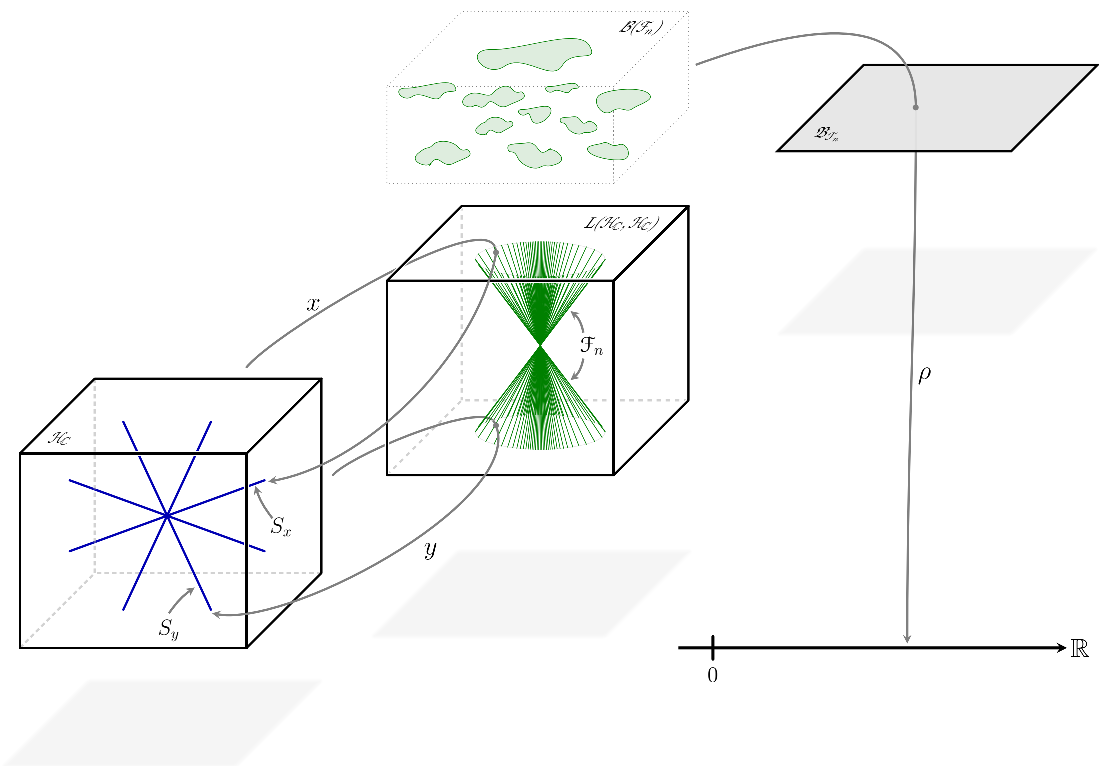

Figure 1.1: Graphical representation of the relation between the structures of a causal fermion system $(\mathcal{H}_\mathbb{C}, \mathcal{F}_n, \rho)$.

$(\mathcal{H}_\mathbb{C}, \langle\cdot|\cdot\rangle_{\mathcal{H}_\mathbb{C}})$ there is the subset $\mathcal{F}_n$ which contains certain finite-rank bounded linear operators which, upon acting on the Hilbert space, trace out so-called spin spaces $S_x, S_y \subset \mathcal{H}_\mathbb{C}$. On top of those two structures there are positive measures which associate a non-negative real number to the elements of the Borel-σ-algebra $\mathcal{B}(\mathcal{F}_n)$. By specifying the Hilbert space $(\mathcal{H}_\mathbb{C}, \langle\cdot|\cdot\rangle_{\mathcal{H}_\mathbb{C}})$ and fixing the spin dimension $n \in \mathbb{N}$, the universal measure ρ remains as the only indeterminate object in the definition. This freedom in the choice of the universal measure is restricted, as will be explained in greater detail below in Section 1.3, by the so-called causal action principle.

In the following subsections, the individual structures occurring in the definition of a causal fermion system and their interrelations are subject of more detailed explanations. To keep the presentation as compact and clear as possible, we agree on the following convention for all further explanations.

Convention 1.1.2

Whenever we refer to the Hilbert space $(\mathcal{H}_\mathbb{C}, \langle\cdot|\cdot\rangle_{\mathcal{H}_\mathbb{C}})$ and the operator set $\mathcal{F}_n$, we tacitly take an underlying causal fermion system $(\mathcal{H}_\mathbb{C}, \mathcal{F}_n, \rho)$ of spin dimension n for granted.

1.1.1 Structuring the Hilbert Space: The Spin Spaces

The combination of a Hilbert space $(\mathcal{H}_\mathbb{C}, \langle\cdot|\cdot\rangle_{\mathcal{H}_\mathbb{C}})$ and the set $\mathcal{F}_n$ consisting of bounded linear operators with finite rank naturally leads to a structuring of the set $\mathcal{H}_\mathbb{C}$ induced by the individual elements of $\mathcal{F}_n \subset \mathrm{L}(\mathcal{H}_\mathbb{C}, \mathcal{H}_\mathbb{C})$.

Definition 1.1.3 (Spin Space and Orthogonal Projection Operator)

For any $x \in \mathcal{F}_n$ the *spin space at $x \in \mathcal{F}_n$* is defined as the image of $\mathcal{H}_\mathbb{C}$ under x

$$\forall x \in \mathcal{F}_n : \; S_x := x(\mathcal{H}_\mathbb{C}) \tag{1.1}$$

The corresponding operator $\pi_x : \mathcal{H}_\mathbb{C} \to S_x$ is referred to as the *orthogonal projection on the spin space S_x*.

Being the image of a finite-rank linear operator, the spin space $S_x \subset \mathcal{H}$ at $x \in \mathcal{F}_n$ naturally is a finite-dimensional complex subvector space of $\mathcal{H}_\mathbb{C}$. As a consequence of this, all spin spaces intersect in $0 \in \mathcal{H}_\mathbb{C}$ as depicted in Figure 1.1. By equipping the individual subvector spaces with indefinite inner products induced by the corresponding finite-rank operator, we obtain so-called *spin inner product spaces.*

Definition 1.1.4 (Spin Inner Product Space)

The *spin inner product space at $x \in \mathcal{F}_n$* is the ordered pair $(S_x, \prec\cdot|\cdot\succ_{S_x})$ where S_x is the spin space at $x \in \mathcal{F}_n$ and where $\prec\cdot|\cdot\succ_{S_x} : S_x \times S_x \to \mathbb{C}$ is the mapping defined as

$$(u_1, u_2) \mapsto \prec u_1|u_2\succ_{S_x} := -\langle u_1|x u_2\rangle_{\mathcal{H}_\mathbb{C}} \tag{1.2}$$

which is referred to as the *spin space inner product on S_x*.

The entirety of all spin inner product spaces can be thought of as forming a structure within the Hilbert space $\mathcal{H}_\mathbb{C}$ which resembles a bristle ball. As will become apparent in Chapter 2 (Modelling Physical Systems in the Framework of Causal Fermion Systems), the spin inner product spaces are the abstract equivalent of fibres of a spinor bundle over physical spacetime.

1.1.2 The Causal Structure of the Operator Set $\mathcal{F}_n$

The elements of the set $\mathcal{F}_n$ not only give rise to an additional subset structure within the underlying Hilbert space, but are interesting objects in their own right: Being linear operators, it is a natural idea to study their eigenvalues. The theory of causal fermion systems, however, is not concerned with the study of the eigenvalues of the operators themselves, but instead builds on the eigenvalues of products xy of operators $x, y \in \mathcal{F}_n$. This characteristic feature of the theory of causal fermion systems lies at the heart of its inherent *non-locality* which will become more explicit in the discussion of the causal action in Section 1.2.

For two arbitrary operators $x, y \in \mathcal{F}_n$, which by definition of $\mathcal{F}_n$ satisfy $\mathrm{rk}(x), \mathrm{rk}(y) \leq 2n$, also their product clearly satisfies $\mathrm{rk}(xy) \leq 2n$. The $2n$ non-trivial[2] eigenvalues of the operator product xy will be denoted by λ_i^{xy} where $i \in \{1, 2, \ldots, 2n\}$. Based on these eigenvalues of operator products, one introduces the following notion of causality on the operator set $\mathcal{F}_n$.[11, Def. 1.1.2]

Definition 1.1.5 (Causal Structure on $\mathcal{F}_n$)

Two operators $x, y \in \mathcal{F}_n$ are called *spacelike-separated* if the eigenvalues $\lambda_i^{xy} \in \mathbb{C}$ of their operator product xy satisfy the condition

$$\exists \lambda^{xy} \in \mathbb{R}_0^+ \ \forall i \in \{1, 2, \ldots, 2n\}\colon \ |\lambda_i^{xy}| = \lambda^{xy} \tag{1.3a}$$

while they are called *timelike-separated* if

$$\forall i \in \{1, 2, \ldots, 2n\}\colon \ \lambda_i^{xy} \in \mathbb{R} \quad \wedge \quad \exists i, j \in \{1, 2, \ldots, 2n\}\colon \ |\lambda_i^{xy}| \neq \left|\lambda_j^{xy}\right| \tag{1.3b}$$

holds. In all other cases the operators x and y are referred to as being *lightlike-separated*.

According to this definition, assessing the causal relation of two operators $x, y \in \mathcal{F}_n$ requires to evaluate and compare the eigenvalues λ_i^{xy} of their operator product. In Section 1.2 we will come back to this definition and introduce the so-called causal Lagrangian, an object that allows for a systematic distinction between spacelike-separated operators $x, y \in \mathcal{F}_n$ on the one hand and timelike-separated as well as lightlike-separated operators on the other hand. Before, however, we introduce another quantity which contains part of the information encoded in the eigenvalues of pairs of operators from $\mathcal{F}_n$.

Definition 1.1.6 (Spectral Weight)

The *spectral weight of an operator* $x \in \mathcal{F}_n$ is the mapping $|\cdot| : \mathcal{F}_n \to \mathbb{R}_0^+$ defined as

$$x \mapsto |x| := \sum_{i=1}^{2n} |\lambda_i^x| \tag{1.4}$$

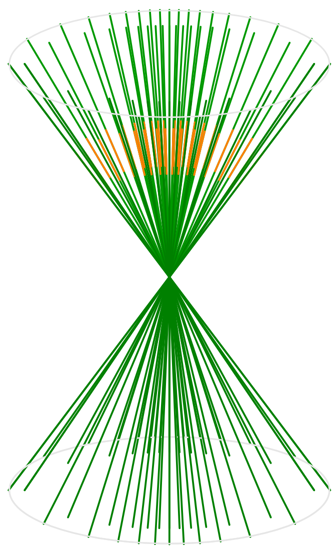

Figure 1.2: Graphical representation of the double-conical set $\mathcal{F}_n$ together with spacetime $M = \mathrm{supp}(\rho)$ associated with a given causal fermion system $(\mathcal{H}_\mathbb{C}, \mathcal{F}_n, \rho)$ depicted in orange.

To conclude this subsection we remark that, although the set of finite-rank operators within $\mathrm{L}(\mathcal{H}_\mathbb{C}, \mathcal{H}_\mathbb{C})$ forms a subvector space due to the fact that linear combinations of finite-rank operators still have finite rank, the subset $\mathcal{F}_n \subset \mathrm{L}(\mathcal{H}_\mathbb{C}, \mathcal{H}_\mathbb{C})$, however, does not have the same property: Since linear combinations $x + y$ for $x, y \in \mathcal{F}_n$ do in general have $\mathrm{rk}(x + y) > 2n$ and thus violate

[2] For convenience, the non-trivial eigenvalues of xy are ordered such that $\lambda_i^{xy} \neq 0$ for $1 \leq i \leq \mathrm{rk}(xy)$ and $\lambda_i^{xy} = 0$ for $\mathrm{rk}(xy) + 1 \leq i \leq 2n$.

the rank condition in the definition of a causal fermion system, $\mathcal{F}_n$ is not a subvector space of $\mathrm{L}(\mathcal{H}_\mathbb{C}, \mathcal{H}_\mathbb{C})$. But since rescalings of $x \in \mathcal{F}_n$ with constants $c \in \mathbb{R} \setminus \{0\}$ do not affect the rank of the operator x, the set $\mathcal{F}_n$ has a structure which is referred to as a *double-conical set.*[12, p. 3] As a consequence, the operator set $\mathcal{F}_n$ may be depicted as an infinite collection of "rays" intersecting at $0 \in \mathcal{F}_n$ as shown in Figure 1.2. For completeness of the discussion, we introduce one more definition.

Definition 1.1.7 (Regular Operators and Regular Causal Fermion Systems)

An operator $x \in \mathcal{F}_n$ is call *regular* if it has rank $2n$. The subset of regular operators is defined as

$$\mathcal{F}_n^{\mathrm{reg}} \coloneqq \{x \in \mathcal{F}_n \,|\, \mathrm{rk}(x) = 2n\} \subset \mathcal{F}_n \tag{1.5}$$

and a causal fermion system is thus called *regular* if $\mathcal{F}_n$ is replaced by $\mathcal{F}_n^{\mathrm{reg}}$ in the definition.

The subset $\mathcal{F}_n^{\mathrm{reg}}$ of regular operators is a dense open subset of $\mathcal{F}_n$ and plays an important role in the modelling of physical systems as will become clear in Subsection 2.2.2.1.[3]

1.1.3 The Universal Measure

While the Hilbert space $(\mathcal{H}_\mathbb{C}, \langle\cdot|\cdot\rangle_{\mathcal{H}_\mathbb{C}})$ and the operator set $\mathcal{F}_n$ can be understood as a rather rigid underlying structure,[4] the universal measure ρ may be interpreted as sitting on top of both but without, at least at this point, being subject to any restrictions, except for being a positive measure on the Borel-σ-algebra $\mathcal{B}(\mathcal{F}_n)$ generated by the elements of the subspace topology $\mathcal{T}_{\mathcal{F}_n}$ with respect to the topological space $(\mathrm{L}(\mathcal{H}_\mathbb{C}, \mathcal{H}_\mathbb{C}), \mathcal{T}_{\|\cdot\|})$. In view of later applications we introduce the following definition.

Definition 1.1.8 (Spacetime associated with a Causal Fermion System)

The *spacetime M associated with a causal fermion system* $(\mathcal{H}_\mathbb{C}, \mathcal{F}_n, \rho)$ is defined as the support of the universal measure

$$M \coloneqq \mathrm{supp}(\rho) \coloneqq \mathcal{F}_n \setminus \bigcup \big\{\Omega \subset \mathcal{F}_n \,\big|\, \Omega \in \mathcal{B}(\mathcal{F}_n) \,\wedge\, \rho(\Omega) = 0\big\} \tag{1.6}$$

The spacetime M associated with a given causal fermion system $(\mathcal{H}_\mathbb{C}, \mathcal{F}_n, \rho)$ corresponds to the orange portion of $\mathcal{F}_n$ in Figure 1.2. Without intending to violate our claim for a clear distinction between the abstract mathematical framework and concrete physical applications, we nevertheless want to mention that the spacetime associated with a causal fermion system is usually a low-dimensional subset of $\mathcal{F}_n$.[5]

1.2 The Causal Lagrangian and the Causal Action

Having expanded on the definition of a causal fermion system and the structures which it is built from, we now come back to the causal structure of the operator set $\mathcal{F}_n$ already addressed in Subsection 1.1.2 and introduce with the so-called *causal Lagrangian* a quantity that allows for a systematic distinction of pairs of spacelike-separated operators.

[3] For a detailed discussion of regular causal fermion systems and, in particular, the Banach manifold structure of $\mathcal{F}_n^{\mathrm{reg}}$ we refer to the recent work by Finster and Lottner.[13]

[4] In this context, "rigidity" refers to the fact that the part $(\mathcal{H}_\mathbb{C}, \mathcal{F}_n)$ of a causal fermion system $(\mathcal{H}_\mathbb{C}, \mathcal{F}_n, \rho)$ is completely determined by specifying two numbers: First, the Hilbert space dimension $\dim(\mathcal{H}_\mathbb{C}) \in \mathbb{N}_0 \cup \{\infty\}$ must be fixed. This effectively amounts to choosing either $\mathcal{H}_\mathbb{C} = \mathbb{C}^{\dim(\mathcal{H}_\mathbb{C})}$ in the finite-dimensional case or $\mathcal{H}_\mathbb{C} = \ell^2(\mathbb{N}, \mathbb{C})$ in the infinite-dimensional setting since every separable Hilbert space is isometrically isomorphic to ℓ^2. Second and finally, by fixing the spin dimension $n \in \mathbb{N}_0$ the universal measure remains as the only undetermined input.

[5] Numerical studies in simple examples such as distributions of points on the sphere demonstrate that the universal measure has its support on low-dimensional elements of $\mathcal{B}(\mathcal{F}_n)$.[8, 14]

Definition 1.2.1 (Causal Lagrangian)

The *causal Lagrangian* is the function $\mathcal{L} : \mathcal{F}_n \times \mathcal{F}_n \to \mathbb{R}_0^+$ defined as

$$(x, y) \mapsto \mathcal{L}(x, y) \overset{(1.4)}{:=} \left|(xy)^2\right| - \frac{1}{2n} \left|xy\right|^2 \tag{1.7}$$

where $\left|(xy)^2\right|$ and $|xy|$ denote the spectral weights of the operators $(xy)^2$ and xy, respectively.

From this abstract representation of the causal Lagrangian its relevance and the mentioned connection with the causal structure on the operator set $\mathcal{F}_n$ cannot be recognized immediately.

1.2.1 Eigenvalue Representation of the Causal Lagrangian

To work out this connection, it is insightful to rewrite the causal Lagrangian, evaluated at the operator pair $(x, y) \in \mathcal{F}_n \times \mathcal{F}_n$, as stated in the following lemma.

Lemma 1.2.2 (Eigenvalue Representation of the Causal Lagrangian)

Let $x, y \in \mathcal{F}_n$ be operators. Then the causal Lagrangian $\mathcal{L}(x, y)$ can be expressed as

$$\mathcal{L}(x, y) = \frac{1}{4n} \sum_{i,j=1}^{2n} \left(\left|\lambda_i^{xy}\right| - \left|\lambda_j^{xy}\right|\right)^2 \tag{1.8}$$

where λ_i^{xy} for $i \in \{1, 2, \ldots, 2n\}$ are the non-trivial eigenvalues of the operator product xy.

Proof. Evaluating the causal Lagrangian at $(x, y) \in \mathcal{F}_n \times \mathcal{F}_n$ and inserting the definition of the spectral weight, we obtain

$$\mathcal{L}(x, y) \overset{(1.7)}{=} \left|(xy)^2\right| - \frac{1}{2n} \left|xy\right|^2 \overset{(1.4)}{=} \sum_{i=1}^{2n} \left|\lambda_i^{(xy)^2}\right| - \frac{1}{2n} \left(\sum_{i=1}^{2n} \left|\lambda_i^{xy}\right|\right)^2$$

To rewrite the first term, we make use of the fact that if λ_i^{xy} is an eigenvalue of the operator xy corresponding to the eigenvector $v \in \mathcal{H}_\mathbb{C}$ one can immediately conclude that the eigenvalue of the operator $(xy)^2$ corresponding to the same eigenvector $v \in \mathcal{H}_\mathbb{C}$ is given by the square of the eigenvalue λ_i^{xy}. Using this argument along with the multiplicativity of the absolute value, we arrive at

$$\mathcal{L}(x, y) = \sum_{i=1}^{2n} \left|\lambda_i^{xy}\right|^2 - \frac{1}{2n} \left(\sum_{i=1}^{2n} \left|\lambda_i^{xy}\right|\right)^2$$

Introducing a factor $1 = \frac{1}{2n} \sum_{j=1}^{2n} 1$ in the first term yields

$$\mathcal{L}(x, y) = \frac{1}{2n} \sum_{i,j=1}^{2n} \left|\lambda_i^{xy}\right|^2 - \frac{1}{2n} \left(\sum_{i=1}^{2n} \left|\lambda_i^{xy}\right|\right) \left(\sum_{j=1}^{2n} \left|\lambda_j^{xy}\right|\right)$$

Finally, by splitting up the first term, interchanging summation indices and completing the square, we end up with an expression in terms of the eigenvalues of the operator product xy

$$\mathcal{L}(x, y) = \frac{1}{4n} \sum_{i,j=1}^{2n} \left|\lambda_i^{xy}\right|^2 - 2 \cdot \frac{1}{4n} \sum_{i,j=1}^{2n} \left|\lambda_i^{xy}\right|\left|\lambda_j^{xy}\right| + \frac{1}{4n} \sum_{i,j=1}^{2n} \left|\lambda_j^{xy}\right|^2 = \frac{1}{4n} \sum_{i,j=1}^{2n} \left(\left|\lambda_i^{xy}\right| - \left|\lambda_j^{xy}\right|\right)^2$$

This concludes the proof. □

In this eigenvalue representation of the causal Lagrangian its already mentioned significance for the assessment of the causal relation of two operators $x, y \in \mathcal{F}_n$ becomes apparent: According to Definition 1.1.5 two operators $x, y \in \mathcal{F}_n$ are spacelike-separated if all eigenvalues of their operator product xy have the same absolute value, which thus immediately implies that for such a pair of operators the causal Lagrangian vanishes identically. Due to this property, the causal Lagrangian can be used in order to identify those subsets within the operator set $\mathcal{F}_n$ whose elements are spacelike-separated from a fixed operator $x \in \mathcal{F}_n$. This usage of the causal Lagrangian will become particularly relevant in Subsection 1.2.2 and Section 1.3.

Interpretation of the Causal Lagrangian

In addition to the usage of the causal Lagrangian as a quantity for the evaluation of the causal relation of two operators $x, y \in \mathcal{F}_n$, another yet not discussed interpretation shall be introduced and explained here. If one defines for a given pair of operators $x, y \in \mathcal{F}_n$ the average absolute value $\lambda_{\mathrm{a}}^{xy} \in \mathbb{R}_0^+$ of all eigenvalues as $\lambda_{\mathrm{a}}^{xy} := \frac{1}{2n} \sum_{i=1}^{2n} \left|\lambda_i^{xy}\right|$ and adds $0 = \lambda_{\mathrm{a}}^{xy} - \lambda_{\mathrm{a}}^{xy}$ in the eigenvalue representation of the causal Lagrangian as derived in Lemma 1.2.2, we obtain

$$\begin{aligned}\mathcal{L}(x, y) &\overset{(1.8)}{=} \frac{1}{4n} \sum_{i,j=1}^{2n} \left(\left|\lambda_i^{xy}\right| - \left|\lambda_j^{xy}\right|\right)^2 = \frac{1}{4n} \sum_{i,j=1}^{2n} \left(\left(\left|\lambda_i^{xy}\right| - \lambda_{\mathrm{a}}^{xy}\right) - \left(\left|\lambda_j^{xy}\right| - \lambda_{\mathrm{a}}^{xy}\right)\right)^2 \\ &= \sum_{i=1}^{2n} \left(\left|\lambda_i^{xy}\right| - \lambda_{\mathrm{a}}^{xy}\right)^2 - \frac{1}{2n} \left(\sum_{i=1}^{2n} \left(\left|\lambda_i^{xy}\right| - \lambda_{\mathrm{a}}^{xy}\right)\right)^2 \end{aligned} \tag{1.9}$$

If one now inserts the definition of $\lambda_{\mathrm{a}}^{xy}$ in the second term, it vanishes identically and we are left with

$$\mathcal{L}(x, y) = \sum_{i=1}^{2n} \left(\left|\lambda_i^{xy}\right| - \lambda_{\mathrm{a}}^{xy}\right)^2 \tag{1.10}$$

In structural terms, this representation of the causal Lagrangian resembles the expression for the variance of a discrete random variable Λ^{xy}, which can take the values $\left|\lambda_i^{xy}\right|$, whose associated probabilities of occurrence are $p_i = \frac{1}{2n}$ for all $i \in \{1, 2, \ldots, 2n\}$. In view of this, the causal Lagrangian may be written as

$$\mathcal{L}(x, y) = 2n \mathrm{Var}(\Lambda^{xy}) \tag{1.11}$$

which allows to interpret the causal Lagrangian, for a fixed pair of operators $x, y \in \mathcal{F}_n$, as a measure of the dispersion of the absolute values of the eigenvalues λ_i^{xy} around the average absolute value $\lambda_{\mathrm{a}}^{xy}$. If one allows for physical parlance, the causal Lagrangian thus corresponds to the one-dimensional moment of inertia of the distribution of the absolute values $\left|\lambda_i^{xy}\right|$ of the non-trivial eigenvalues of two operators $x, y \in \mathcal{F}_n$ with respect to their average absolute value $\lambda_{\mathrm{a}}^{xy}$.

1.2.2 The Causal Action

Having introduced the definition of the causal Lagrangian along with a discussion of its meaning, we now come to the main object in the theory of causal fermion systems.

Definition 1.2.3 (Causal Action)

Let $\mathfrak{B}_{\mathcal{F}_n}$ denote the positive Borel measures on the measurable space $(\mathcal{F}_n, \mathcal{B}(\mathcal{F}_n))$ introduced in Definition 1.1.1. The *causal action* is the function $\mathcal{S} : \mathfrak{B}_{\mathcal{F}_n} \to \mathbb{R}_0^+$ defined as

$$\rho \mapsto \mathcal{S}(\rho) \overset{(1.7)}{:=} \iint_{\mathcal{F}_n \times \mathcal{F}_n} \mathcal{L}(x, y) \, \mathrm{d}\rho(x) \, \mathrm{d}\rho(y) \tag{1.12}$$

where $\mathcal{L}(x, y)$ and ρ denote the causal Lagrangian and the universal measure, respectively.

Interpretation of the Causal Action

Considering the measure $\rho \in \mathfrak{B}_{\mathcal{F}_n}$ as a prescription which assigns a certain weight to elements of the Borel-σ-algebra $\mathcal{B}(\mathcal{F}_n)$ and taking into account that the causal Lagrangian gives information on the causal relation[6] of two operators $x, y \in \mathcal{F}_n$, the causal action can thus be understood as a nonlocal, ρ-dependent device to quantify the total causal relations of *all* the operators contained in $\operatorname{supp}(\rho) \subset \mathcal{F}_n$. For a given Hilbert space $(\mathcal{H}_\mathbb{C}, \langle\cdot|\cdot\rangle_{\mathcal{H}_\mathbb{C}})$ and fixed spin dimension n, the causal action thus provides a possibility to assign a numerical value to different causal fermion systems $(\mathcal{H}_\mathbb{C}, \mathcal{F}_n, \rho)$ which takes into account the causal structure on $\mathcal{F}_n$ in the sense that spacelike-separated operators do not give a contribution.

1.3 The Causal Action Principle

The objects introduced in Section 1.1 and Section 1.2 form the skeleton of the theory of causal fermion systems and allow for a classification of causal fermion systems according to the real number $\mathcal{S}(\rho)$ assigned to a universal measure ρ via the causal action. In order to introduce some kind of dynamics, however, it is not sufficient to only assign numerical values to universal measures, but instead one has to specify which numerical value for $\mathcal{S}(\rho)$ is desirable. Only by designating a distinguished value for $\mathcal{S}(\rho)$ it is possible to *rate* and not only *classify* different universal measures.

Definition 1.3.1 (Causal Action Principle)

The *causal action principle* consists in minimizing the causal action by varying the universal measure ρ within the class of regular[a] Borel measures $\mathfrak{B}^{\text{reg}}_{\mathcal{F}_n}$ on the measurable space $(\mathcal{F}_n, \mathcal{B}(\mathcal{F}_n))$ under the following constraints:

(1) *Volume Constraint:* For any choice of the universal measure $\rho \in \mathfrak{B}^{\text{reg}}_{\mathcal{F}_n}$, the total volume $\rho(\mathcal{F}_n)$ corresponding to $\mathcal{F}_n \in \mathcal{B}(\mathcal{F}_n)$ has to be kept fixed

$$\forall \rho \in \mathfrak{B}^{\text{reg}}_{\mathcal{F}_n}: \qquad \rho(\mathcal{F}_n) = \text{const} > 0 \tag{1.13a}$$

(2) *Trace Constraint:* For any choice of the universal measure $\rho \in \mathfrak{B}^{\text{reg}}_{\mathcal{F}_n}$, the $\operatorname{tr}_{\mathcal{H}_\mathbb{C}}$-weighted volume of $\mathcal{F}_n$ has to be kept fixed

$$\forall \rho \in \mathfrak{B}^{\text{reg}}_{\mathcal{F}_n}: \qquad \int\limits_{\mathcal{F}_n} \operatorname{tr}_{\mathcal{H}_\mathbb{C}}(x)\, \mathrm{d}\rho(x) = \text{const} \tag{1.13b}$$

(3) *Boundedness Constraint:* For any choice of the universal measure $\rho \in \mathfrak{B}^{\text{reg}}_{\mathcal{F}_n}$, the squared spectral weight of the operator product xy (which equals the first term in the causal Lagrangian) must be bounded from above

$$\forall \rho \in \mathfrak{B}^{\text{reg}}_{\mathcal{F}_n}: \qquad \iint\limits_{\mathcal{F}_n \times \mathcal{F}_n} |xy|^2\, \mathrm{d}\rho(x)\mathrm{d}\rho(y) \leq C \tag{1.13c}$$

[a] We remark that a measure μ defined on a measurable space (X, Σ) where Σ is a σ-algebra on the topological space $(X, \mathcal{T})$ is called *regular*[15, § 52] if every $\Omega \in \Sigma$ is both an inner regular set with respect to μ

$$\forall \Omega \in \Sigma: \quad \mu(\Omega) = \sup\{\mu(A) \,|\, A \subset \Omega \,\wedge\, A \in \Sigma \,\wedge\, A \,\text{compact}\}$$

as well as an outer regular set with respect to μ

$$\forall \Omega \in \Sigma: \quad \mu(\Omega) = \inf\{\mu(B) \,|\, B \supset \Omega \,\wedge\, B \in \Sigma \,\wedge\, B \in \mathcal{T}\}$$

By requiring to vary the universal measure such that the causal action is minimized, this definition distinguishes zero as the desirable value for the causal action and thus allows to rate different choices of the universal measure ρ for given $(\mathcal{H}_\mathbb{C}, \mathcal{F}_n)$.

[6] In the sense that it vanishes for spacelike-separated operators $x, y \in \mathcal{F}_n$.

Interpretation of the Causal Action Principle
As discussed in the paragraph after the definition of a causal fermion system, the universal measure ρ can a priori be chosen arbitrarily without any restrictions. As a consequence of the ρ-dependence of the causal action and through the causal action principle, however, the universal measure can no longer be chosen freely but instead becomes the central variable which is dynamically determined through the interplay of conflicting tendencies: While the prescription to minimize the causal action clearly favours universal measures whose support is chosen such that the contribution to the causal action coming from spacelike-separated pairs of operators is maximized, the constraints counterbalance this tendency and guarantee that trivial minimizers are excluded. As soon as a minimizing measure $\rho_{\min}$ is found, it automatically determines the spacetime associated with the corresponding causal fermion system $(\mathcal{H}_{\mathbb{C}}, \mathcal{F}_n, \rho_{\min})$.

1.3.1 Significance and Interpretation of the Constraints

Having briefly discussed the interpretation of the causal action principle itself, we now focus on the significance and interpretation of the associated constraints which have a two-fold function: First, they guarantee that the causal action principle is *well-posed* in the sense of the direct method in the calculus of variations[16, Sec. 39] and, secondly, that trivial minimizers are ruled out.

Volume Constraint The fact that the constraints are necessary in order to rule out trivial choices for the universal measure can be seen particularly easily from the volume constraint: Without the requirement $\rho(\mathcal{F}_n) = \text{const} > 0$ one could simply choose $\rho \equiv 0$ for the universal measure and thus trivially arrange that $\mathcal{S}(\rho) = 0$ which is clearly pointless.

Trace Constraint If the universal measure is not allowed to vanish everywhere, one could alternatively come up with the idea to construct the universal measure such that its support is at least as small as possible. Choosing ρ as the Dirac measure which is supported at[11, p. 3/4]

$$x = (\underbrace{1, 1, \dots, 1}_{n \text{ times}}, \underbrace{-1, -1, \dots, -1}_{n \text{ times}}, 0, 0, \dots) \in \mathcal{F}_n$$

we find that the causal action collapses to

$$\mathcal{S}(\rho) = \mathcal{L}(x, x) = \frac{1}{4n} \sum_{i,j=1}^{2n} \left(\left|\lambda_i^{xx}\right| - \left|\lambda_j^{xx}\right| \right)^2$$

But since the operator product $xx = (1, 1, \dots, 1, 0, 0, \dots)$ has $2n$ unit entries, all eigenvalues λ_i^{xx} of this operator product coincide which, in turn, makes the causal action vanish. Finally, by suitably rescaling the Dirac measure, one has constructed a trivial minimizer of the causal action which is not ruled out by the volume constraint. In order to avoid also such situations, the trace constraint is necessary.

Boundedness Constraint While the meaning of the above volume and trace constraint may be summarized as a condition on the *size* of the support of the universal measure which, in a sense, must not be "too small", the boundedness constraint is of a different nature. To see this, we first rewrite the boundedness constraint in terms of the eigenvalues of the operator product xy in the same way as in Lemma 1.2.2 and subsequently express the sum of absolute values of the eigenvalues through the average $\lambda_{\mathrm{a}}^{xy}$ which yields

$$\iint\limits_{\mathcal{F}_n \times \mathcal{F}_n} \left|xy\right|^2 \mathrm{d}\rho(x)\mathrm{d}\rho(y) \overset{(1.4)}{=} \iint\limits_{\mathcal{F}_n \times \mathcal{F}_n} \left(\sum_{i=1}^{2n} \left|\lambda_i^{xy}\right| \right)^2 \mathrm{d}\rho(x)\mathrm{d}\rho(y) = (2n)^2 \iint\limits_{\mathcal{F}_n \times \mathcal{F}_n} \left(\lambda_{\mathrm{a}}^{xy}\right)^2 \mathrm{d}\rho(x)\mathrm{d}\rho(y)$$

In order for this expression to be bounded by some finite constant $C > 0$, neither the whole support of the universal measure, nor non-null subsets of it are allowed to "run away" to infinity[7] which suggests to interpret the boundedness constraint as a condition on the *dispersion* of the support of the universal measure.

[7]This is basically the same situation as in Exercise 13.4 (i) of the Online Course on Causal Fermion Systems.

1.3.2 Existence Theory

For the sake of completeness, we shall at least briefly address the question whether, and under what conditions minimizers of the causal action principle exist at all. In the so-called *finite-dimensional setting*, namely for causal fermion systems $(\mathcal{H}_{\mathbb{C}}, \mathcal{F}_n, \rho)$ where the Hilbert space dimension $\dim(\mathcal{H}_{\mathbb{C}})$ and the total volume $\rho(\mathcal{F}_n)$ are both finite, minimizers exist as was proven by Finster.[7] Unlike one would expect, also in the so-called *infinite-dimensional setting* where $\dim(\mathcal{H}_{\mathbb{C}}) = \infty$ and $\rho(\mathcal{F}_n) = \infty$, the causal action principle is still well-posed if one replaces the in this case obviously meaningless volume constraint by the requirement that for two measures $\rho, \tilde{\rho}$ the total volume difference $(\rho - \tilde{\rho})(\mathcal{F}_n)$ vanishes and that the so-called *total variation*[17, Sec. 6.1],[15, § 29] $|\rho - \tilde{\rho}|(\mathcal{F}_n)$ *of the difference of two measures* is finite.[8] The question concerning the existence of minimizers in this setting, however, has not been settled yet, although there are recent existence results in the so-called *non-compact setting*[18, Sec. 2.1] by Finster and Langer.[19],[20] In physically relevant settings which will be discussed in the following Chapter 2 and under the assumption that the regularized kernel of the fermionic projector is homogeneous, minimizers exist also in the infinite-dimensional setting.[7, Ch. 4] In contrast with the finite-dimensional and infinite-dimensional setting, the causal action principle is ill-posed already from the outset if the dimension of the Hilbert space is infinite while the total volume is finite.

1.4 Further Structures and Objects

The essence of the causal action principle presented in the previous section is to adjust the weighting of elements of the Borel-σ-algebra $\mathcal{B}(\mathcal{F}_n)$ for a given Hilbert space $(\mathcal{H}_{\mathbb{C}}, \langle\cdot|\cdot\rangle_{\mathcal{H}_{\mathbb{C}}})$ and operator set $\mathcal{F}_n$ through the universal measure ρ such that the causal action is minimized. This being said, the question arises how the eigenvalues λ_i^{xy} of products of pairs of operators $x, y \in \mathcal{F}_n$ which serve as the building blocks of the causal Lagrangian and thus play a central role in the whole framework, can actually be computed in a systematic and efficient way.

1.4.1 The Kernel of the Fermionic Projector and the Closed Chain

To answer the question concerning a systematic computation procedure for the eigenvalues of an operator product xy of any two operators $x, y \in \mathcal{F}_n$, we make use of the fact that for $x, y \in \mathcal{F}_n$ also the product operator xy satisfies the rank condition $\mathrm{rk}(xy) \leq 2n$. This implies that for any pair $x, y \in \mathcal{F}_n$ the Hilbert space $\mathcal{H}_{\mathbb{C}}$ can be orthogonally decomposed as follows

$$\mathcal{H}_{\mathbb{C}} = I_{xy} \oplus \ker(xy) \tag{1.14}$$

where $I_{xy} \subset \mathcal{H}_{\mathbb{C}}$ is the finite-dimensional sub-vector space which is mapped to itself by xy. If one now defines the operator $xy|_{I_{xy}} : I_{xy} \to I_{xy}$ restricted to this finite-dimensional subspace I_{xy}, its eigenvalues coincide with the nontrivial eigenvalues of the original operator xy. By introducing two mappings between spin spaces, referred to as the *kernel of the fermionic projector* and the *closed chain*, this reasoning can be extended to an efficient algorithm to compute the nontrivial eigenvalues of operator products xy for arbitrary $x, y \in \mathcal{F}_n$.

Definition 1.4.1 (Kernel of the Fermionic Projector)

Let S_x and S_y be the spin spaces at $x \in \mathcal{F}_n$ and $y \in \mathcal{F}_n$, respectively. The *kernel of the fermionic projector* is the mapping $P(x,y) : S_y \to S_x$ defined as

$$u \mapsto \big[P(x,y)\big](u) \coloneqq (\pi_x y|_{S_y})(u) \tag{1.15}$$

where $\pi_x : \mathcal{H}_{\mathbb{C}} \to S_x$ is the orthogonal projection on the spin space S_x while $y|_{S_y} : S_y \to S_y$ denotes the restriction of the operator $y \in \mathcal{F}_n$ to the (finite-dimensional) spin space S_y.[a]

[a]The restricted operator $y|_{S_y} : S_y \to S_y$ is defined by $u \mapsto y|_{S_y}(u) \coloneqq yu$ for all $u \in S_y$.

[8]The latter condition actually means that the two measures may differ at most on a set of finite volume. For a more in-depth discussion we refer to the work by Finster and Kleiner.[18, Sec. 2.1]

From this operator, by interchanging arguments and taking the composition, the following operator can be constructed which will eventually allow to compute the sought-after eigenvalues λ_i^{xy}.

Definition 1.4.2 (Closed Chain)

Let S_x and S_y again be the spin spaces at $x \in \mathcal{F}_n$ and $y \in \mathcal{F}_n$, respectively. The *closed chain* is the mapping $A_{xy} : S_x \to S_x$ defined in terms of the kernel of the fermionic projector as

$$u \mapsto A_{xy}(u) \overset{(1.15)}{:=} \big[P(x,y)P(y,x)\big](u) \tag{1.16}$$

Using this closed chain which is an endomorphism of the finite-dimensional spin space S_x, we can now establish a relation between its eigenvalues and the eigenvalues of the operator product xy for $x, y \in \mathcal{F}_n$ in the following way:[11, p. 5/6] We start by rewriting the Hilbert space trace $\mathrm{tr}_{\mathcal{H}_\mathbb{C}}$ of the operator product $(xy)^p$ for arbitrary $p \geq 1$ by exploiting the cyclicity of the trace as

$$\mathrm{tr}_{\mathcal{H}_\mathbb{C}}\left((xy)^p\right) = \mathrm{tr}_{\mathcal{H}_\mathbb{C}}\left(x(yx)^{p-1}y\right) = \mathrm{tr}_{\mathcal{H}_\mathbb{C}}\left((yx)^{p-1}yx\right) = \mathrm{tr}_{\mathcal{H}_\mathbb{C}}\left((yx)^p\right)$$

Now, since $x \in \mathcal{F}_n$ satisfies $\mathrm{rk}(x) \leq 2n$ by definition, the trace on the right-hand side reduces to

$$\mathrm{tr}_{\mathcal{H}_\mathbb{C}}\left((yx)^p\right) = \sum_{i\in\mathbb{N}} \langle e_i | (yx)^p e_i \rangle_{\mathcal{H}_\mathbb{C}}$$

where $(e_i)_{i\in\mathbb{N}}$ is a basis of the separable Hilbert space $\mathcal{H}_\mathbb{C}$. This result can be reproduced if one instead considers the closely related operator $\pi_x (yx)^p|_{S_x} : S_x \to S_x$ and takes the ordinary trace Tr_{S_x} on the (finite-dimensional) spin space S_x. We thus arrive at

$$\mathrm{tr}_{\mathcal{H}_\mathbb{C}}\left((yx)^p\right) = \mathrm{Tr}_{S_x}\left(\pi_x (yx)^p|_{S_x}\right)$$

Next, we have to establish the connection between the operator $\pi_x (yx)^p|_{S_x}$ and the closed chain A_{xy} which both are defined on the finite-dimensional spin space S_x. To this end, we take the closed chain to the p^{th} power and compute

$$\begin{aligned}
(A_{xy})^p &\overset{(1.16)}{=} \left((\pi_x y|_{S_y})(\pi_y x|_{S_x})\right)^p = \left(\pi_x y \pi_y x|_{S_x}\right)^p = \underbrace{[\pi_x (y\pi_y) x|_{S_x}] \dots [\pi_x (y\pi_y) x|_{S_x}]}_{p \text{ times}} \\
&= \pi_x \underbrace{\{(y\pi_y)(x|_{S_x}\pi_x)\} \dots \{(y\pi_y)(x|_{S_x}\pi_x)\}}_{(p-1) \text{ times}} (y\pi_y) x|_{S_x} = \pi_x (y\pi_y x \pi_x)^{p-1} y(\pi_y) x|_{S_x} \\
&= \pi (yx)^p|_{S_x}
\end{aligned}$$

where for the second and fifth equality we used the definition of the restricted operators $y|_{S_y}$ and $x|_{S_x}$, respectively, while for the last equality we exploited the relations $y\pi_y = y$ and $x\pi_x = x$.[9] This demonstrates that for all $p \geq 1$ the Hilbert space trace of powers of the operator product xy can equivalently be computed by taking the trace of the p^{th} power of the closed chain A_{xy} on the finite-dimensional spin space S_x

$$\mathrm{tr}_{\mathcal{H}_\mathbb{C}}\left((xy)^p\right) = \mathrm{Tr}_{S_x}\left(A_{xy}^p\right)$$

With this result at hand, it only remains to remark that the coefficients of both the characteristic polynomial of the operator product xy as well as the characteristic polynomial of the closed chain A_{xy} can be expressed in terms of combinations of traces of powers of xy and A_{xy}, respectively. Thus, we conclude that the eigenvalues of operator products xy for arbitrary operators $x, y \in \mathcal{F}_n$ (acting on the possibly infinite-dimensional Hilbert space $\mathcal{H}_\mathbb{C}$) can equivalently, but much more conveniently be computed from the closed chain A_{xy} which acts on the always at least $2n$-dimensional spin space S_x.

[9] This holds due to the fact that for self-adjoint operators their image and kernel are orthogonal.

Adjoint of the Kernel of the Fermionic Projector

Having equipped the spin spaces with an inner product which led to the spin inner product spaces, it is natural to study the adjoint of the kernel of the fermionic projector with respect to the inner products introduced in Definition 1.1.4. In view of the definition of the kernel of the fermionic projector as a mapping $P(x,y) : S_y \to S_x$ between finite-dimensional inner product spaces $(S_y, \prec\cdot|\cdot\succ_{S_y})$ and $(S_x, \prec\cdot|\cdot\succ_{S_x})$, its adjoint clearly is a mapping $P(x,y)^* : S_x \to S_y$ defined by the relation

$$\forall u \in S_x \, \forall v \in S_y : \quad \prec P(x,y)^* u|v\succ_{S_y} = \prec u|P(x,y)v\succ_{S_x} \tag{1.17}$$

As a consequence of the definition of the spin space inner product, the kernel of the fermionic projector and its adjoint are related in the following way.

Proposition 1.4.3 (Symmetry of the Kernel of the Fermionic Projector)

The kernel of the fermionic projector and its adjoint $P(x,y)^*$ are related via

$$P(x,y)^* = P(y,x) \tag{1.18}$$

which is usually referred to as *symmetry of the kernel of the fermionic projector*.

Proof. The symmetry of the kernel of the fermionic projector essentially traces back to the self-adjointness of the building blocks of $P(x,y)$ with respect to the Hilbert space inner product: Inserting $P(x,y) = \pi_x y|_{S_y}$ into (1.17) and making use of the definition of the spin space inner product on S_x, we find for arbitrary $u \in S_x$ and $v \in S_y$

$$\begin{aligned} \prec P(x,y)^* u|v\succ_{S_y} &\overset{(1.17)}{=} \prec u|P(x,y)v\succ_{S_x} \underset{(1.15)}{\overset{(1.2)}{=}} -\langle u|x\pi_x y|_{S_y} v\rangle_{\mathcal{H}_\mathbb{C}} = -\langle u|xyv\rangle_{\mathcal{H}_\mathbb{C}} \\ &= -\langle xu|yv\rangle_{\mathcal{H}_\mathbb{C}} = -\langle \pi_y xu|\pi_y yv\rangle_{\mathcal{H}_\mathbb{C}} = -\langle \pi_y x|_{S_x} u|yv\rangle_{\mathcal{H}_\mathbb{C}} \\ &\underset{(1.15)}{\overset{(1.2)}{=}} \prec P(y,x)u|v\succ_{S_y} \end{aligned} \tag{1.19}$$

where for the third equality we used the relation $x\pi_x = x$ together with the definition of the restricted operator, while for the sixth equality we employed the identity $y = \pi_y y$ along with the self-adjointness of π_y.

This concludes the proof. □

1.4.2 Wavefunctions and the Wave Evaluation Operator

Besides the kernel of the fermionic projector and the closed chain, which both are of particular importance for explicitly calculating the eigenvalues of products xy for arbitrary operators $x, y \in \mathcal{F}_n$, there are further objects which become relevant in concrete physical applications which will be discussed in the following chapter.

Definition 1.4.4 (Wavefunction)

A *wavefunction* is a mapping $\psi : M \to \mathcal{H}_\mathbb{C}$ which satisfies the condition

$$\forall x \in M : \psi(x) \in S_x \tag{1.20}$$

where M denotes the spacetime associated with a causal fermion system $(\mathcal{H}_\mathbb{C}, \mathcal{F}_n, \rho)$.

This definition does not specify the functional dependence of $\psi(x)$ on $x \in M$. By employing the orthogonal projection on S_x, however, there is a natural way in which every element of the Hilbert space gives rise to a unique wavefunction.

Definition 1.4.5 (Physical Wavefunction)

The *physical wavefunction of* $u \in \mathcal{H}_\mathbb{C}$ is the wavefunction $\psi^u : M \to \mathcal{H}_\mathbb{C}$ defined as

$$x \mapsto \psi^u(x) := \pi_x u \tag{1.21}$$

In order to complete the definition of physical wavefunctions to a coherent overall picture, we introduce one further mapping which to each element of the Hilbert space $\mathcal{H}_\mathbb{C}$ assigns the corresponding physical wavefunction.

Definition 1.4.6 (Wave Evaluation Operator)

The *wave evaluation operator* is the mapping $\Psi : \mathcal{H}_\mathbb{C} \to C(M, SM)$ defined as

$$u \mapsto \Psi(u) := \psi^u \tag{1.22}$$

where $C(M, SM)$ denotes the set of continuous wavefunctions.[a]

[a] We remark that a wavefunction ψ is continuous at $x \in M$ if it satisfies

$$\forall \varepsilon > 0 \, \exists \delta > 0 \, \forall y \in M \text{ with } \|y - x\| < \delta : \; \left\| |y|^{1/2}\psi(y) - |x|^{1/2}\psi(x) \right\|_{\mathcal{H}_\mathbb{C}} < \varepsilon$$

where $|x|^{1/2}$ denotes the square root of the absolute value[21, p. 196] $|x| := (x^*x)^{1/2}$ of the operator $x \in M$.[11, p. 8]

These objects are the most relevant ones for this thesis. As already mentioned in the introduction to this chapter, the intensive work on the theory of causal fermion systems in different directions during the past two decades has led to a variety of structures and objects which appear in different contexts and can be grouped into *inherent structures* and *analytic structures*.

Inherent Structures

When talking about so-called *inherent structures*, one means structures which exclusively require information already encoded in the data $\mathcal{H}_\mathbb{C}, \mathcal{F}_n$ and ρ which together define a causal fermion system. This category includes all the objects introduced in this chapter, namely spin spaces, the kernel of the fermionic projector, the closed chain as well as the wavefunction and the wave evaluation operator. Besides these structures there are the following:

- *Geometric Structures* Starting from symmetric linear endomorphisms of spin spaces, one introduced so-called *Clifford extensions* which in turn allow to define tangent spaces to spin spaces. Building on this, a spin connection as well as notions of curvature and parallel transport can be developed for causal fermion systems of spin dimension $n = 2$.[22] The corresponding investigations in case $n = 1$ are currently being conducted by Saeed Zafari.

- *Topological Structures* Complementary to the above differential geometric constructions, causal fermion systems also contain topological information which was analyzed for the first time by Finster and Kamran.[23]

- *Surface Layer Integrals* In the study of symmetries and conservation laws in the framework of causal fermion systems, the concept of so-called *surface layer integrals* which are double-integrals of short-range causal Lagrangian over “thickened” surfaces, were introduced by Finster and Kleiner.[24]

Analytic Structures

Besides these structures and objects there are also *analytic structures* which include *Euler-Lagrange equations*, *linearized field equations*, the *surface layer one-form*, the *symplectic form* as well as the *surface layer inner product* where the latter three are formulated using surface layer integrals. For a continuously updated overview we refer to the website on the theory of causal fermion systems.

2

Modelling Physical Systems in the Framework of Causal Fermion Systems

Contents

In the previous chapter we introduced the fundamental mathematical structures of the theory of causal fermion systems and explained their mutual interrelationship. Except for some physically-inspired terminology we have paid particular attention not to establish any content-wise connection to physics in order to maintain a clear distinction between the abstract mathematical structures of the theory of causal fermion systems on the one hand, and the description of concrete physical systems *within* this framework on the other hand. In this chapter we now address the latter question, namely how physical systems can be modelled within the mathematical structures provided by the theory of causal fermion systems. In Section 2.1 we start by discussing the foundational conceptions which underlie the modelling, before in Section 2.2 we give a detailed explanation how $(\mathcal{H}_{\mathbb{C}}, \langle\cdot|\cdot\rangle_{\mathcal{H}_{\mathbb{C}}})$, $(\mathcal{F}_n, \mathcal{B}(\mathcal{F}_n))$ and ρ have to be chosen in order to model spacetimes described by Lorentzian manifolds. The resulting regularized analogues of all the objects introduced in Sections 1.2 to 1.4 will serve as the starting point for the considerations in Part II. In the final Section 2.3 we specialize to the Minkowski vacuum and derive an explicit expression for the iε-regularized causal Lagrangian which will be needed in Part III.

2.1 Foundational Conceptions underlying the Modelling

The initial question in the development of a physical theory aimed at describing nature is to decide, usually based at least in part on measurements and experiments, which objects, structures and principles one considers as being fundamental. Due to our principally incomplete knowledge concerning the very essence of nature, this decision is inevitably subjective and, at least to a certain degree, reflects the currently prevailing physical paradigms.[25] Before we enlarge on the foundational conceptions underlying the modelling approach in the context of causal fermion systems, we introduce the following terminology.

Terminology 2.1.1 (Physical System)

In what follows, the term *physical system* always means some physical spacetime[a] together with all the particle and antiparticle content existing therein. Accordingly, a *physical vacuum system* is a physical system without any particles or antiparticles present.

[a] To avoid potential confusion caused by the notion of spacetime $M = \operatorname{supp}(\rho)$ as the support of the universal measure ρ, we will always add the qualifier "physical" when talking about the inseparable fabric of space and time from our everyday experience which is mathematically modelled as a possibly curved, semi-Riemannian manifold.

Having specified what is meant when talking about physical systems, we now turn to the foundational conceptions underlying the modelling of physical systems within the framework of causal fermion systems, which are basically the following three:

(1) Fermions as the Fundamental Building Blocks The experimental observation from high-energy physics that all fundamental matter particles in the standard model of particle physics are fermions while the interaction particles have bosonic character, leads to the plausible but nevertheless *subjective* conception that the different fermion species[1] should be regarded as the fundamental building blocks of a physical theory.[26, p. 11]

(2) Dirac Sea Interpretation of Negative-Energy Solutions The Feynman-Stückelberg interpretation of the negative-energy solutions of the Dirac equation in quantum electrodynamics is withdrawn and replaced by its predecessor, namely the Dirac sea interpretation, according to which the total absence of particles and antiparticles (of one species) must be understood as presence of the entirety of all negative-energy Dirac solutions (of this species).

While these first two conceptions are of course subjective, but nevertheless well-motivated from and supported by experimental evidence, the third conception is quite different: Taking the conceptual incompatibility of general relativity and quantum field theories as the starting point[26, p. 7], it postulates a new feature of spacetime at small length scales.

(3) Microscopic Structure of Physical Spacetime The ultraviolet divergences in quantum field theory suggest to assume that physical spacetime has some non-trivial structure on microscopic length scales which is implemented by modifying the small-scale behaviour of solutions of the Dirac equation and considering these *regularized* objects as being the fundamental ones.[11, p. 15]

As will be explained further below in Subsection 2.2.2, it is this third item, namely the proposed existence of some unknown but physically real microstructure of physical spacetime which together with the causal action principle and the associated mathematical structures introduced in Chapter 1 is the main novelty of the theory of causal fermion systems. Before we further enlarge on the

[1] When talking about *fermion species*, we refer to the elementary spin-1/2-particles in the standard model of particle physics, namely the six quarks (u, d, c, s, t, b) and six leptons $(e, \mu, \tau, \nu_e, \nu_\mu, \nu_\tau)$ which are usually organized in three so-called *generations* (u, d, e, ν_e), (c, s, μ, ν_μ), (t, b, τ, ν_τ), each consisting of one up-type and down-type quark as well as of one charged and one neutral lepton.

modelling of physical systems based on the above conceptions, however, we have to discuss the Dirac sea interpretation of the negative-energy solutions of the Dirac equation in order to account for the fact that it is both subject to ongoing discussions with the regular conclusion of being an outdated and overruled concept, but at the same time is of central importance for our modelling.

The Dirac Sea Interpretation

The whole discussion traces back to the year 1928 when Dirac generalized Schrödinger's equation in order arrive at a wave equation which respects both the principles of quantum mechanics as well as those of special relativity. Although this development was in principle highly desirable and marks a great success, it came at the price of suddenly having to deal with a whole bunch of previously absent negative-energy solutions – along with the necessity for a clear physical interpretation of these experimentally unobserved solutions. In order to resolve this obvious discrepancy between theoretical predictions and experimental observations, Dirac employed the exclusion principle[27] formulated some years earlier by the Austrian physicist Wolfgang Pauli, and proposed the following *"solution of the negative energy difficulty"*:[28, § 2]

> *"The most stable states for an electron (i. e. the states of lowest energy) are those with negative energy and very high velocity. All the electrons in the world will tend to fall into these states with emission of radiation. The Pauli exclusion principle, however, will come into play and prevent more than one electron going into any one state. Let us assume there are so many electrons in the world that all the most stable states are occupied, or, more accurately, that all the states of negative energy are occupied except perhaps a few of small velocity. Any electrons with positive energy will now have very little chance of jumping into negative-energy states and will therefore behave like electrons are observed to behave in the laboratory. We shall have an infinite number of electrons in negative-energy states, and indeed an infinite number per unit volume all over the world, but if their distribution is exactly uniform we should expect them to be completely unobservable. Only the small departures from exact uniformity, brought about by some of the negative-energy states being unoccupied, can we hope to observe."*

Although Dirac in those days incorrectly concluded that one is *"led to the assumption that the holes in the distribution of negative-energy electrons are protons"*, the idea of complete occupation of all states of negative energy soon became known as the *Dirac sea.*[2] During the development of quantum electrodynamics, Dirac's interpretation was superseded by the Feynman-Stückelberg interpretation according to which negative-energy solutions of the Dirac equation should be re-interpreted as positive-energy solutions propagating backwards in time.

Although quantum electrodynamics is without any doubt an excellent theory and has significantly shaped our current understanding of nature due to the extremely accurate agreement of theoretically predicted and experimentally measured values of quantities such as the anomalous magnetic moment of the electron (also known as the Landé factor) or the Lamb shift in the hydrogen atom, its success still does not logically rule out the older Dirac sea interpretation.[3] In sharp contrast with these results, the discovery of a discrepancy between the theoretically calculated and experimentally measured decay rate of the neutral pion π^0 which was later explained by Adler[34], Bell and Jackiw[35] and became known as the chiral anomaly of quantum electrodynamics, indeed suggests a quite different conclusion: As is nicely explained by Jackiw[36, p. 5-8], it is *"[...] the negative energy sea [which] is responsible for nonconservation of chirality even though the dynamics is chirally invariant"*. Based on this he argues that *"[...] we must assign physical reality to Dirac's*

[2] Although Dirac's identification of the vacant states with protons was wrong, the correct explanation of *"duplexity phenomena"* as he called the discrepancy between the experimentally observed and theoretically predicted number of stationary states of an electron in an atom,[29] led to the discovery of the *"positive electron"*, now referred to as the positron, in 1932 by Anderson[30] and consequently a correction in later publications by Dirac.[31],[32]

[3] In this context, we shall not miss to point to an interesting discussion by Finster (in its original version in German[5, Sec. 1.4] but later, in a slightly revised version, also available in English[33, Ch. 7]), where he argues that the above-mentioned precision tests of quantum electrodynamics are not really suitable to justify the concept of field quantization.

negative energy sea, because it produces the chiral anomaly, whose effects are experimentally observed, principally in the decay of the neutral pion to two photons, but there are other physical consequences as well."[36, p. 8],[37, p. 12] This brief comparison demonstrates that, although the Feynman-Stückelberg interpretation is now widely considered as the favoured interpretation which is due to the enormous success of quantum field theories, the situation is much more ambiguous than it appears at first sight. In fact, the whole situation strikingly resembles the interpretational problems which arose from Einstein's explanation of the photoelectric effect and, later, from de Broglie's wave hypothesis roughly one century ago: In much the same way as the wave-particle duality serves as a placeholder for our ignorance regarding the real nature of what in some cases we conceive as particles but as waves at other times, the yet unanswered question concerning the actual nature of the entirety of negative-energy solutions of the Dirac equation may analogously be referred to as the *fermionic vacuum state duality.* Given this ambiguous situation, we opt for Dirac's original interpretation and model physical systems based on this assumption.

2.2 Modelling Physical Vacuum Systems

Having discussed the three foundational conceptions which underlie the modelling of physical systems within the framework of causal fermion systems, we now explain in detail how to construct a causal fermion system which models a given physical system. In order to clearly work out how and where the foundational conceptions enter the construction such that there do not remain any conceptual gaps, we deliberately decided to proceed in small steps. Furthermore, as the thesis may be considered as part of the groundwork for a novel mechanism to explain baryogenesis within the theory of causal fermion systems, we restrict attention to the modelling of physical *vacuum* systems.

2.2.1 The Hilbert Space of Negative-Energy Dirac Solutions

Modelling a given physical system within the structures provided by the theory of causal fermion systems means to find a *concrete realization* of the structures $(\mathcal{H}_{\mathbb{C}}, \langle \cdot | \cdot \rangle_{\mathcal{H}_{\mathbb{C}}})$, $(\mathcal{F}_n, \mathcal{B}(\mathcal{F}_n))$ and $\rho : \mathcal{B}(\mathcal{F}_n) \to \mathbb{R}_0^+$ which together form a causal fermion system $(\mathcal{H}_{\mathbb{C}}, \mathcal{F}_n, \rho)$, thereby taking into account the foundational conceptions. According to the definition of a causal fermion system, the first decision concerns the question how to choose the all-underlying Hilbert space $(\mathcal{H}_{\mathbb{C}}, \langle \cdot | \cdot \rangle_{\mathcal{H}_{\mathbb{C}}})$. Following up on the discussion in the paragraph on the Dirac sea interpretation, we make the following foundational assumption.

Assumption 2.2.1 (Physical Vacuum System corresponds to One Dirac Sea)

In order to implement the first and second item on the list of foundational conceptions, we equate a physical vacuum system with one completely filled Dirac sea corresponding to one of the elementary fermionic particle species in the standard model of particle physics. This means that the Hilbert space $(\mathcal{H}_{\mathbb{C}}, \langle \cdot | \cdot \rangle_{\mathcal{H}_{\mathbb{C}}})$ has to be chosen such that it contains all the negative-energy solutions of the Dirac equation (for this particle species) in the respective physical spacetime under consideration.[a]

[a] We would like to emphasize that the structure of a causal fermion system as introduced in Definition 1.1.1 does in no way suggest, nor require or even enforce this particular choice of the Hilbert space. It is only the *subjective* conviction that the unobserved entirety of negative-energy solutions of the Dirac equation should be interpreted as a Dirac sea which leads to this choice.

This assumption, namely to equate a physical vacuum system with only *one* Dirac sea, oversimplifies the physical reality as the following remark shows.

Remark 2.2.2 (Number of Dirac Seas for Realistic Physical Vacuum System)

A *full* implementation of the first and second item on the list of foundational conceptions would have required to equate a physical vacuum system with a total of 24 completely filled Dirac seas, each corresponding to one of the different elementary fermionic particle species (counting the three different *color charges* of the six quarks) in the standard model of particle physics.[a]

[a]We remark that the number of 24 Dirac seas comes about as follows: As the quarks come in three different "versions" corresponding to the three colors charges, we need a total of eight Dirac seas to model the first generation (u, d, e, ν_e), namely each three copies for the up-quark u and down-quark d as well as each one Dirac sea for the electron e and the associated neutrino ν_e. Including also the other two generations by prolonging u, d, e and ν_e to so-called *families* (u, c, t), (d, s, b), (e, μ, τ) and $(\nu_e, \nu_\mu, \nu_\tau)$, we end up with the necessity for in total 24 Dirac seas.[6, Sec. 2.3, 5.1]

The above assumption is realized by first constructing the Hilbert space $(\mathcal{H}_m, (\cdot|\cdot)_m)$ of *all* solutions of the Dirac equation of mass $m \in \mathbb{R}_0^+$ in the physical spacetime under consideration[4] and subsequently choosing $(\mathcal{H}, \langle\cdot|\cdot\rangle_{\mathcal{H}})$ as the closed subspace of negative-energy solutions with the corresponding Hilbert space inner product being the restriction $\langle\cdot|\cdot\rangle_{\mathcal{H}} := (\cdot|\cdot)_m|_{\mathcal{H}\times\mathcal{H}}$ of $(\cdot|\cdot)_m : \mathcal{H}_m \times \mathcal{H}_m \to \mathbb{C}$ to $\mathcal{H} \times \mathcal{H}$.[5] Although the procedure appears clear at first sight, a closer inspection reveals that there are several technical difficulties which call for closer inspection.[6]

Construction of the Hilbert Space $(\mathcal{H}_m, (\cdot|\cdot)_m)$

As our whole modelling approach is based on solutions of the Dirac equation, the first task is to specify the underlying physical spacetime. Although explicit calculations in all following chapters will exclusively take place in Minkowski space $(\mathscr{M}, \eta)$, we nevertheless sketch the construction of the all-underlying Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle_{\mathcal{H}})$ representing the Dirac sea in the more general case where physical spacetime is described by some smooth Lorentzian manifold $(\mathscr{M}, g)$ which, at least up to this point, is not subject to any restrictions.

The Guiding Principle The natural starting point for the construction of the Hilbert space $(\mathcal{H}_m, (\cdot|\cdot)_m)$ of solutions of the Dirac equation in some general smooth Lorentzian manifold $(\mathscr{M}, g)$ is clearly Minkowski space $(\mathscr{M}, \eta)$: Here the Cauchy problem for given smooth initial data localized in some compactly-supported region on, say, the hypersurface $\{(x^0, \vec{x}) \in \mathscr{M} \mid x^0 = 0\}$, exhibits a unique global solution which, by exploiting the fact that the coefficients of the Dirac operator are constant, can be straightforwardly constructed using the method of Fourier transforms. As soon as Minkowski space $(\mathscr{M}, \eta)$ is replaced by some general smooth Lorentzian manifold $(\mathscr{M}, g)$, however, this method does no longer apply which is due to the fact that the coefficients of the Dirac operator are not constant any more. In order to still be able to construct a unique solution to the Dirac equation for given smooth initial data localized in some compactly-supported region of physical spacetime, we have to restrict the initial freedom in the choice of the smooth Lorentzian manifold $(\mathscr{M}, g)$ by imposing additional geometric assumptions.[7]

The Necessity of Global Hyperbolicity Without intending to enter a detailed discussion at this point, we remark that the necessary geometric assumption which is required to carry over the idea to split physical spacetime into something as *space* and *time* in the first place and subsequently construct a unique global solution of the Dirac equation in a smooth Lorentzian manifold for some prescribed initial data localized in a compactly-supported subset at some initial time, is to impose *global hyperbolicity*[40, Def. 1.3.8] of the Lorentzian manifold $(\mathscr{M}, g)$[38, Sec. 3.5]. If we furthermore assume $\mathscr{M}$ to be time-oriented, it can be shown that physical spacetime $\mathscr{M}$ admits a smooth foliation $\mathscr{M} = (\mathscr{N}_t)_{t\in\mathbb{R}}$ which can be chosen such that $\mathscr{N}_t := \{t\} \times \mathscr{N}$ is a smooth,

[4]Since, according to our current knowledge, we live in a spacetime which is mathematically best modeled as a four-dimensional Lorentzian manifold locally looking like Minkowski space, we will restrict our attention to this class of spacetimes.

[5]We reserve the notation $(\mathcal{H}_{\mathbb{C}}, \langle\cdot|\cdot\rangle_{\mathcal{H}_{\mathbb{C}}})$ for an abstract Hilbert space and denote a concrete realization by $(\mathcal{H}, \langle\cdot|\cdot\rangle_{\mathcal{H}})$.

[6]We follow the presentation by Finster and Jokel[26, Sec. 2.5], enriched with additional material from a yet not published introductory textbook by Finster, Kleiner and Treude.[38, Sec. 3.5]

[7]For a detailed treatment of Cauchy problems for Dirac operators, we refer to chapter 4 in the book on *Wave Equations on Lorentzian Manifolds* by Bär et al.[39, Ch. 4] which is also available as a free online version.[40, Ch. 3] By employing Leray's results[41, Ch. 3] along with the Lichnerowicz-Weitzenböck formula which establishes a relation between the Dirac operator and the Laplace-Beltrami operator, existence of fundamental solutions of the Dirac equation in Lorentzian manifolds can also be shown as described by Dimock[42, Thm. 2.1].

spacelike Cauchy hypersurface in $\mathscr{M}$.[40, Thm. 1.3.10], [8] Moreover, by restricting attention to four-dimensional Lorentzian manifolds the existence of spin structures is ensured[45] and thus allows to define the geometric Dirac operator as

$$\mathcal{D} : \Gamma^\infty(\mathscr{M}, S\mathscr{M}) \to \Gamma^\infty(\mathscr{M}, S\mathscr{M}) \quad \text{with} \quad \psi \mapsto \mathcal{D}\psi := \mathrm{i}\gamma^j \nabla_j \psi \tag{2.1}$$

which acts on smooth sections $\Gamma^\infty(\mathscr{M}, S\mathscr{M})$ of the spinor bundle $\pi : S\mathscr{M} \to \mathscr{M}$ with fibres $\pi^{-1}(x) := S_x\mathscr{M} \simeq \mathbb{C}^4$ carrying an indefinite inner product $\prec \cdot \,|\, \cdot \succ_{S_x\mathscr{M}} : S_x\mathscr{M} \times S_x\mathscr{M} \to \mathbb{C}$ of signature $(2,2)$ referred to as *spinor space inner product*. In the above definition ∇ denotes the metric connection on the spinor bundle which is induced via the Levi-Civita connection ∇_g on the tangent bundle. Furthermore, Clifford multiplication is described by the mapping $\gamma : T_x\mathscr{M} \to \mathrm{L}(S_x\mathscr{M}, S_x\mathscr{M})$ which satisfies the anticommutation relation

$$\gamma(u)\gamma(v) + \gamma(v)\gamma(u) = 2g(u,v)\mathrm{id}_{S_x\mathscr{M}} \tag{2.2}$$

and is written in components using the Dirac matrices γ^j. In this setting and under the assumption of global hyperbolicity, the Cauchy problem for the Dirac equation with mass $m \in \mathbb{R}_0^+$, namely the task to find solutions $\psi \in \Gamma^\infty(\mathscr{M}, S\mathscr{M})$ of

$$(\mathcal{D} - m)\psi = 0 \qquad \text{under} \qquad \psi|_{\mathscr{N}_{t_0}} = \psi_0 \in \Gamma(\mathscr{N}_{t_0}, S\mathscr{M}) \tag{2.3}$$

is now well-posed. Even more, due to the finite speed of propagation for solutions of hyperbolic partial differential equations such as the Dirac equation, initial data $\psi_0 \in \Gamma^\infty_{\mathrm{sc}}(\mathscr{N}_{t_0}, S\mathscr{M})$ with compact support on a (spacelike) Cauchy hypersurface $\mathscr{N}_{t_0}$ evolve into solutions $\psi \in \Gamma^\infty_{\mathrm{sc}}(\mathscr{N}_t, S\mathscr{M})$ with compact support on any other Cauchy hypersurface $\mathscr{N}_t$.

Inner Product on Solutions of the Dirac Equation Again, by analogy with Minkowski space[9], we can define an inner product $(\cdot|\cdot)_m : \Gamma^\infty_{\mathrm{sc}}(\mathscr{N}_t, S\mathscr{M}) \times \Gamma^\infty_{\mathrm{sc}}(\mathscr{N}_t, S\mathscr{M}) \to \mathbb{C}$ for solutions $\psi, \phi \in \Gamma^\infty_{\mathrm{sc}}(\mathscr{N}_t, S\mathscr{M})$ of the Dirac equation as the integral over the (spacelike) Cauchy hypersurface $\mathscr{N}_t$ (with future-directed normal ν) with respect to the Borel measure corresponding to the Riemannian volume form induced by the Lorentzian volume form $\mathrm{d}V_g$ as

$$(\psi|\phi)_m := 2\pi \int_{\mathscr{N}_t} \mathrm{d}\mu_{\mathscr{N}_t}(\vec{x}) \; \prec\phi|\nu_i\gamma^i\phi\succ_{S_x\mathscr{M}} \tag{2.4}$$

where $\prec\cdot|\cdot\succ_{S_x\mathscr{M}} : S_x\mathscr{M} \times S_x\mathscr{M} \to \mathbb{C}$ denotes the indefinite inner product on the fibre $\pi^{-1}(x) = S_x\mathscr{M}$ defined above. Finally, by forming the completion of $\Gamma^\infty_{\mathrm{sc}}(\mathscr{N}_t, S\mathscr{M})$ with respect to the inner product $(\cdot|\cdot)_m$, we arrive at the Hilbert space $(\mathcal{H}_m, (\cdot|\cdot)_m)$ of solutions of the Dirac equation where

$$\mathcal{H}_m := \overline{\left\{\psi \in \Gamma^\infty_{\mathrm{sc}}(\mathscr{M}, S\mathscr{M}) \,\middle|\, (\mathcal{D} - m)\psi = 0\right\}}^{(\cdot|\cdot)_m} \tag{2.5}$$

Choice of the Closed Subspace $(\mathcal{H}, \langle\cdot|\cdot\rangle_{\mathcal{H}})$
Having outlined the construction of the Hilbert space of *all* solutions of the Dirac equation with spatially compact support in a globally hyperbolic, time-oriented smooth Lorentzian manifold $(\mathscr{M}, g)$, the question remains how to implement the Dirac sea interpretation, namely how to identify the subspace corresponding to the negative-energy solutions. Just as before, it is instructive to first consider the problem in Minkowski space: As already mentioned above and as will be discussed further below in Subsection 2.3.1, the solutions of the Dirac equation in Minkowski space are plane waves. This allows for a natural splitting of the whole solution space $\mathcal{H}_m$ into two subspaces

[8] In more basic terms, the underlying theorems are the so-called *splitting theorem* due to Geroch[43, Thm. 11] and the results obtained by Bernal and Sánchez.[44, Thm. 1.1]

[9] Recall that in Minkowski space every solution ψ of the Dirac equation gives rise to a divergence-free *Dirac current* $j^k := \prec\psi|\gamma^k\psi\succ_{S_x\mathscr{M}}$. By using current conservation one finds that the spatial integral over $\prec\psi|\gamma^0\psi\succ_{S_x\mathscr{M}}$ is time-independent and thus allows to define a time-independent inner product by exploiting the polarization identity for complex vector spaces.

according to the sign of the frequency in the Fourier exponential which, via Planck's constant, are interpreted as the positive-energy and negative-energy solutions of the (free) Dirac equation. In the generalized setting discussed above, however, this possibility fails just as Fourier methods fail for the construction of solutions. Nevertheless, by making use of the so-called *fermionic signature operator* introduced by Finster and Reintjes[46, Sec. 3.3] along with the *mass oscillation property*[47] one can define a canonical splitting of the Hilbert space of all Dirac solutions into two subspaces also in globally hyperbolic spacetimes. Since the main part of this thesis is concerned with causal fermion systems modelling Minkowski space, we do not want to go into further detail.

2.2.2 The Set of Operators and the Regularized Universal Measure

By choosing the Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle_{\mathcal{H}})$ as described above, we not only fixed one of the structures necessary to determine a causal fermion system, but we also implemented the first and second item on our list of foundational conceptions. This being said, it remains to answer the questions how the set $\mathcal{F}_n$ of operators has to be chosen in this setting and, moreover, how the conception that physical spacetime should carry some non-trivial microstructure is incorporated.

Informal Discussion To answer these questions, we recall from Section 1.3 that the causal action principle is to vary the universal measure for a given Hilbert space $(\mathcal{H}_{\mathbb{C}}, \langle\cdot|\cdot\rangle_{\mathcal{H}_{\mathbb{C}}})$ and operator set $\mathcal{F}_n$ such that the causal action is minimized. In this way, namely by adjusting the weighting assigned to the elements in $\mathcal{B}(\mathcal{F}_n)$ by ρ such that $\mathcal{S}(\rho)$ is minimized, a certain measure $\rho_{\min}$ is singled out which, in turn, determines some distinguished subset $\operatorname{supp}(\rho_{\min}) \subset \mathcal{F}_n$. In short, the causal action principle boils down to an abstract mechanism that distinguishes certain operators within $\mathcal{F}_n$. Now, if one wants to model a physical system within the structures provided by the theory of causal fermion systems including the conception that physical spacetime has some non-trivial microstructure, the above described mechanism can be used to determine this yet unknown microstructure: In much the same way as the Einstein-Hilbert action along with the principle of least action may be understood as a mechanism to single out metrics which are *"optimal"* in the sense that they minimize the weighted scalar curvature of physical spacetime, the causal action principle determines microstructures of physical spacetime which are *"optimal"* in the sense that they minimize the weighted causal relations between physical spacetime points. In order to implement this idea, the information on the non-trivial microstructure of physical spacetime $\mathscr{M}$ must be encoded into the universal measure which requires to introduce a mapping

$$\mathrm{F}^{\varepsilon} : \mathscr{M} \to \mathcal{F}_n \tag{2.6}$$

and subsequently define ρ^{ε} as the pushforward $\rho^{\varepsilon} := \mathrm{F}^{\varepsilon}_{*}\mu$ of the measure μ on physical spacetime $\mathscr{M}$.

2.2.2.1 Construction of the Local Correlation Function

Having motivated the necessity for a mapping $\mathrm{F}^{\varepsilon} : \mathscr{M} \to \mathcal{F}_n$ which allows to represent the non-trivial microstructure of physical spacetime $\mathscr{M}$ on the operator set $\mathcal{F}_n$, we now explain how to construct this mapping. Taking the second and third item on our list of foundational conceptions as the starting point, the information on the non-trivial microstructure must be extracted solely from the elements of the Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle_{\mathcal{H}})$ of negative-frequency solutions of the Dirac equation. In order to be able to formalize this properly, we first have to introduce so-called *regularization operators*.[11, Def. 1.2.3]

Definition 2.2.3 (Regularization Operator)

A *family of regularization operators* is a family $(\mathfrak{R}^{\varepsilon})_{\varepsilon\in(0,\varepsilon_{\max})}$ of linear operators

$$\mathfrak{R}^{\varepsilon} : \mathcal{H} \to \Gamma(\mathscr{M}, S\mathscr{M}) \tag{2.7}$$

which map the Hilbert space $\mathcal{H}$ to the set of continuous sections of the spinor bundle $\pi : S\mathscr{M} \to \mathscr{M}$ and satisfy the following conditions:

(1) Pointwise Boundedness of $\mathfrak{R}^\varepsilon(\mathcal{H})$: For every member $\mathfrak{R}^\varepsilon$ of the family $(\mathfrak{R}^\varepsilon)_{\varepsilon\in(0,\varepsilon_{\max})}$, the image $\mathfrak{R}^\varepsilon(\mathcal{H}) \subset \Gamma(\mathscr{M}, S\mathscr{M})$ is *pointwise* bounded[a]

$$\forall \varepsilon \in (0, \varepsilon_{\max})\, \forall x \in \mathscr{M}\, \exists C > 0,\ \forall u \in \mathcal{H} : \ \big|\big(\mathfrak{R}^\varepsilon u\big)(x)\big| \leq C\|u\|_{\mathcal{H}} \tag{2.8a}$$

where $|\cdot|$ is any pointwise norm on the spinor spaces.[b]

(2) Almost-everywhere Equicontinuity of $\mathfrak{R}^\varepsilon(\mathcal{H})$: For every member $\mathfrak{R}^\varepsilon$ of the family $(\mathfrak{R}^\varepsilon)_{\varepsilon\in(0,\varepsilon_{\max})}$, the subset $\mathfrak{R}^\varepsilon(\mathcal{H}) \subset \Gamma(\mathscr{M}, S\mathscr{M})$ is equicontinuous *almost everywhere*[c]

$$\begin{aligned}\forall \varepsilon \in (0, \varepsilon_{\max})\, \forall x \in (\mathscr{M} \setminus \mathscr{N})\, \forall \delta > 0\, \exists U \in \mathcal{T}_{\mathscr{M}} \text{ with } x \in U,\ \forall u \in \mathcal{H}\, \forall y \in U :\\ \big|\big(\mathfrak{R}^\varepsilon u\big)(x) - \big(\mathfrak{R}^\varepsilon u\big)(y)\big| \leq \delta\|u\|_{\mathcal{H}}\end{aligned} \tag{2.8b}$$

(3) Weak Convergence to the Identity: In the limit $\varepsilon \to 0$ the family $(\mathfrak{R}^\varepsilon)_{\varepsilon\in(0,\varepsilon_{\max})}$ converges weakly to the identity mapping

$$\begin{aligned}\forall \mathscr{K} \subset \mathscr{M} \text{ compact } \forall \delta > 0\, \exists \varepsilon_0 > 0,\ \forall \varepsilon \in (0, \varepsilon_0)\, \forall u \in \mathcal{H}\, \forall \eta \in C_0^\infty(\mathscr{K}, S\mathscr{M}) :\\ \left| \int_{\mathscr{M}} \prec \eta(x) | \big(\mathfrak{R}^\varepsilon u - u\big)(x) \succ_{S_x\mathscr{M}}\ \mathrm{d}^4x \right| \leq \delta \|u\|_{\mathcal{H}} |\eta|_{C^1(\mathscr{K})}\end{aligned} \tag{2.8c}$$

[a]For clarity, we remark that in this context *pointwise* clearly refers to the "points" in $\mathcal{H}$. The pointwise bound $C(u) > 0$ is realized as $C(u) = C\|u\|_{\mathcal{H}}$.

[b]The first choice is to make use of the inner product $(\cdot|\cdot)_m$ introduced in (2.4) by setting $|\cdot|^2 := (\cdot|\cdot)_m$. However, other choices are equally possible.

[c]Without having explicitly mentioned it, we assume a given measure space $(\mathscr{M}, \mathcal{B}(\mathscr{M}), \mu)$ where $\mathscr{N} \in \mathcal{B}(\mathscr{M})$ is an element of the σ-algebra $\mathcal{B}(\mathscr{M})$ satisfying $\mu(\mathscr{N}) = 0$.

The significance of these regularization operators is that they cure an unwanted but inevitable feature of the Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle_{\mathcal{H}})$ which is due to construction: As the Hilbert space $\mathcal{H}_m$ is obtained by taking the completion of the set of solutions $\psi \in \Gamma^\infty_{\text{sc}}(\mathscr{M}, S\mathscr{M})$ of the Dirac equation, its elements cannot be expected to be continuous functions; instead, since smooth, compactly supported functions are dense in L^2, the elements of $\mathcal{H}_m$ are merely L^2-functions upon restriction to arbitrary Cauchy hypersurfaces. But since regularized Dirac solutions as the fundamental physical objects should at least be continuous functions according to our subjective conviction, the regularization operators map the Hilbert space $\mathcal{H}$ to $\Gamma(\mathscr{M}, S\mathscr{M})$. As a consequence, for any $\psi \in \mathcal{H}$ the object $\mathfrak{R}^\varepsilon\psi \in \Gamma(\mathscr{M}, S\mathscr{M})$ can be evaluated pointwise and thus allows for the following definition which for any pair $\psi_1, \psi_2 \in \mathcal{H}$ provides information on the correlation of their regularized counterparts at the physical spacetime point $x \in \mathscr{M}$.

Definition 2.2.4 (Regularized Sesquilinear Form on $(\mathcal{H}, \langle\cdot|\cdot\rangle_{\mathcal{H}})$)

Let $(\mathcal{H}, \langle\cdot|\cdot\rangle_{\mathcal{H}})$ be the Hilbert space constructed in Subsection 2.2.1. For any $x \in \mathscr{M}$ the regularized sesquilinear form $b_x^\varepsilon : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ is defined in terms of the spinor space inner product $\prec \cdot | \cdot \succ_{S_x\mathscr{M}} : S_x\mathscr{M} \times S_x\mathscr{M} \to \mathbb{C}$ on the fibres of the spinor bundle $(S\mathscr{M}, \pi, \mathscr{M})$ as

$$(u, v) \mapsto b_x^\varepsilon(u, v) := - \prec (\mathfrak{R}^\varepsilon u)(x) | (\mathfrak{R}^\varepsilon v)(x) \succ_{S_x\mathscr{M}} \tag{2.9}$$

Before we proceed, note that $b_x^\varepsilon : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ is well-defined as a sesquilinear form on $\mathcal{H}$ due to the fact that regularization operators $\mathfrak{R}^\varepsilon : \mathcal{H} \to \Gamma(\mathscr{M}, S\mathscr{M})$ are by definition linear and the spinor space inner product $\prec \cdot | \cdot \succ_{S_x\mathscr{M}} : S_x\mathscr{M} \times S_x\mathscr{M} \to \mathbb{C}$ introduced after (2.1) is an inner product on the fibres of the spinor bundle $\pi : S\mathscr{M} \to \mathscr{M}$ which are four-dimensional complex vector spaces. Using this sesquilinear form, we can now establish a connection between regularized elements of $\mathcal{H}$ which can be thought of as representing negative-energy solutions of the Dirac equation with a modified behaviour on microscopic length scales, and the operator set $\mathcal{F}_n$.

Lemma 2.2.5 (Sesquilinear Form gives rise to Local Correlation Operator)

For any $x \in \mathscr{M}$, the regularized sesquilinear form $b_x^\varepsilon : \mathcal{H}\times\mathcal{H} \to \mathbb{C}$ on the Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle_\mathcal{H})$ gives rise to a bounded linear operator $\mathrm{F}^\varepsilon(x) : \mathcal{H} \to \mathcal{H}$, referred to as *local correlation operator*, which has at most two positive and at most two negative eigenvalues and allows to express the sesquilinear form in terms of the Hilbert space inner product $\langle\cdot|\cdot\rangle_\mathcal{H} : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ as

$$\forall u, v \in \mathcal{H} : \qquad b_x^\varepsilon(u, v) = \langle u|\mathrm{F}^\varepsilon(x)v\rangle_\mathcal{H} \tag{2.10}$$

Proof. To begin with, we remark that evaluating a regularization operator $\mathfrak{R}^\varepsilon : \mathcal{H} \to \Gamma(\mathscr{M}, S\mathscr{M})$ at $x \in \mathscr{M}$ yields, by definition, a linear mapping $(\mathfrak{R}^\varepsilon(\,\cdot\,))(x) : \mathcal{H} \to S_x\mathscr{M}$. Due to the fact that the spinor spaces $S_x\mathscr{M}$ are four-dimensional complex vector spaces, the operator $(\mathfrak{R}^\varepsilon(\,\cdot\,))(x)$ is actually a finite-rank operator on $\mathcal{H}$. Furthermore, by recalling that the mapping $(\mathfrak{R}^\varepsilon(\,\cdot\,))(x) : \mathcal{H} \to S_x\mathscr{M}$ is pointwise bounded and by using the Cauchy-Schwarz inequality, we can conclude that b_x is a bounded sesquilinear form on $\mathcal{H}$.

As a consequence of this, the mapping $b_x^\varepsilon(\,\cdot\,, v) : \mathcal{H} \to \mathbb{C}$ is a bounded, conjugate-linear form on $\mathcal{H}$ and thus an element of the continuous dual space $\mathcal{H}^*$ for any choice of $v \in \mathcal{H}$. Now, by the Fréchet-Riesz representation theorem there is a uniquely determined element $w \in \mathcal{H}$ such that the continuous conjugate-linear functional $b_x^\varepsilon(\,\cdot\,, v) \in \mathcal{H}^*$ can be expressed in terms of the Hilbert space inner product as

$$\forall u \in \mathcal{H} : \qquad b_x^\varepsilon(u, v) = \langle u|w\rangle_\mathcal{H} \tag{2.11}$$

By making use of the linearity of the sesquilinear form b_x in its second argument, we conclude that w must depend linearly on the choice of v. Furthermore, in order to ensure that the right-hand side in the above defining equation is bounded, the linear operator which maps v to w must be bounded. Finally, by including the x-dependence, we find that the sesquilinear form b_x^ε can be described by a bounded linear operator $\mathrm{F}^\varepsilon(x) : \mathcal{H} \to \mathcal{H}$ as

$$\forall u, v \in \mathcal{H} : \qquad b_x^\varepsilon(u, v) = \langle u|\mathrm{F}^\varepsilon(x)v\rangle_\mathcal{H} \tag{2.12}$$

Taking into account that b_x^ε is defined in terms of an indefinite inner product of signature $(2, 2)$, the operator $\mathrm{F}^\varepsilon(x)$ must both be self-adjoint (with respect to the Hilbert space inner product $\langle\cdot|\cdot\rangle_\mathcal{H}$) and of rank at most four with at most two positive and at most two negative eigenvalues. Thus, by choosing spin dimension $n = 2$, we have $\mathrm{F}^\varepsilon(x) \in \mathcal{F}_2$ for all $x \in \mathscr{M}$.

This concludes the proof. □

Definition 2.2.6 (Local Correlation Function)

For any $\varepsilon \in (0, \varepsilon_{\max})$ the function $\mathrm{F}^\varepsilon : \mathscr{M} \to \mathcal{F}_2$ which is defined in terms of regularization operators and the spinor space inner product as

$$\forall u, v \in \mathcal{H} : \qquad \langle u|\mathrm{F}^\varepsilon(x)v\rangle_\mathcal{H} \overset{(2.9)}{\underset{(2.10)}{:=}} -\prec(\mathfrak{R}^\varepsilon u)(x)|(\mathfrak{R}^\varepsilon v)(x)\succ_{S_x\mathscr{M}} \tag{2.13}$$

is referred to as the *local correlation function*.

2.2.2.2 The Regularized Universal Measure

Having introduced the local correlation function which establishes a relation between physical spacetime $\mathscr{M}$ and the operator set $\mathcal{F}_2$, we are finally in the position to specify how to choose the universal measure in order to finally obtain a causal fermion system which models a Lorentzian manifold without particles and antiparticles.

Definition 2.2.7 (Regularized Universal Measure)

Let $(\mathscr{M}, g)$ be a smooth, oriented Lorentzian manifold, let

$$\mathrm{d}V_g = |\det(g)|^{1/2}\mathrm{d}x^1 \wedge \cdots \wedge \mathrm{d}x^{\dim(\mathscr{M})} \tag{2.14}$$

denote the Lorentzian volume form in a given chart and let $\mu_g : \mathcal{B}(\mathscr{M}) \to \mathbb{R}_0^+$ be the Lebesgue-Borel measure corresponding to the volume form.[a] Then the *regularized universal measure* is defined as the pushforward measure $\rho^\varepsilon : \mathcal{B}(\mathcal{F}_2) \to \mathbb{R}_0^+$ of μ_g defined as[11, eq. (1.2.5)]

$$\Omega \mapsto \rho^\varepsilon(\Omega) := (\mathrm{F}^\varepsilon_* \mu_g)(\Omega) := \mu_g\big((\mathrm{F}^\varepsilon)^{-1}(\Omega)\big) \qquad \forall \Omega \in \sigma(\mathrm{F}^\varepsilon) \subset \mathcal{B}(\mathcal{F}_2) \tag{2.15}$$

where $\sigma(\mathrm{F}^\varepsilon) := \{(\mathrm{F}^\varepsilon)^{-1}(A) \,|\, A \in \mathcal{B}(\mathscr{M})\}$ denotes the σ-algebra generated by the local correlation function.

[a]Note that the terminology *Lebesgue-Borel measure* has been chosen to indicate that the Lebesgue measure has to be restricted to the Borel sets in order ensure compatibility with the definition of a causal fermion system. For details on the Lebesgue measure corresponding to the volume form, we refer to the presentation in the book by Amann and Escher.[48, Ch. 12]

Taking together all the ingredients, namely the Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle_{\mathcal{H}})$ as constructed in Subsection 2.2.1, as well as the operator set $\mathcal{F}_2$ and the regularized universal measure ρ^ε which both rely on the local correlation function, we end up with a family of causal fermion system $(\mathcal{H}, \mathcal{F}_2, \rho^\varepsilon)$[10] which model a Lorentzian manifold without any particles or antiparticles present, but with a non-trivial microstructure of physical spacetime on the length scale ε.

2.2.3 Further Regularized Objects

With the definition of the local correlation function at hand, we can now study how the spin spaces, the kernel of the fermionic projector and the closed chain as introduced in Subsection 1.1.1 and Subsection 1.4.1, respectively, are *realized* in this setting. In order to maintain the distinction between the structures of the theory of causal fermion systems and the modelling of a concrete physical system within these structures, we introduce the following notation and terminology.

Terminology 2.2.8 (Regularized Objects)

In what follows, elements of the Lorentzian manifold $(\mathscr{M}, g)$ are consistently denoted by $x, y, z \in \mathscr{M}$ in order to distinguish them from operators $x, y, z \in \mathcal{F}_2$. Furthermore, whenever an object depends on the chosen microstructure of physical spacetime via the local correlation function F^ε, we add a superscript $(\,\cdot\,)^\varepsilon$ to indicate the dependence on the regularization.[a]

[a]For clarity, we remark that the superscript $(\,\cdot\,)^\varepsilon$ is meant to encode both information on the *type* of regularization as well as on the *length scale* of the regularization, which is also denoted by ε.

2.2.3.1 Regularized Spin Spaces

Starting from the causal fermion system $(\mathcal{H}, \mathcal{F}_2, \rho^\varepsilon)$ constructed in the previous subsection, we now explain how the spin spaces are realized in this setting.

Definition 2.2.9 (Regularized Spin Spaces)

For any $x \in \mathscr{M}$ the *regularized spin space* S_x^ε *at* $x \in \mathscr{M}$ is defined as the spin space at $\mathrm{F}^\varepsilon(x) \in \mathcal{F}_2$. More explicitly, the regularized spin space S_x^ε at $x \in \mathscr{M}$ is given by

[10]We remark that, as introduced by Oppio[49, Def. 4.9], it is reasonable to refer to the pair $(\mathcal{H}, \mathrm{F}^\varepsilon_* \mu_g)$ as the *regularized causal fermion system (of* $\mathcal{H}$*)* since the Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle_{\mathcal{H}})$ together with the regularization encoded in the local correlation function F^ε and the given measure μ_g completely determine the causal fermion system.

$$\forall x \in \mathscr{M} : \; S_x^\varepsilon := S_{F^\varepsilon(x)} \overset{(1.1)}{=} \big[F^\varepsilon(x)\big](\mathcal{H}) \tag{2.16}$$

Together with the *regularized spin space inner product on* S_x^ε which by analogy with Definition 1.1.4 is the mapping $\prec \cdot | \cdot \succ_{S_x^\varepsilon} : S_x^\varepsilon \times S_x^\varepsilon \to \mathbb{C}$ defined as

$$\forall u_1, u_2 \in S_x^\varepsilon : \; \prec u_1 | u_2 \succ_{S_x^\varepsilon} := -\langle u_1 | F^\varepsilon(x) u_2 \rangle_{\mathcal{H}} \tag{2.17}$$

we arrive at the *regularized spin inner product space* $(S_x^\varepsilon, \prec \cdot | \cdot \succ_{S_x^\varepsilon})$ *at* $x \in \mathscr{M}$. The operator $\pi_{F^\varepsilon(x)} : \mathcal{H} \to S_x^\varepsilon$ is referred to as the *orthogonal projection on the regularized spin space* S_x^ε.

Remark 2.2.10 (Regularized Spin Spaces)

The fact that the subset $S_x^\varepsilon \subset \mathcal{H}$ contains elements which are originally constructed from Dirac spinors, one could argue to better use the terminology "regularized *spinor* space". But since a given physical system is modelled within the structures of the theory of causal fermion systems and not the other way round, it is more consistent to refer to S_x^ε as regularized spin spaces.

2.2.3.2 The Regularized Kernel of the Fermionic Projector

Having introduced regularized spin spaces as the concrete realizations of the spin spaces in our setting where the causal fermion system is given by $(\mathcal{H}, \mathcal{F}_2, \rho^\varepsilon)$, we can define the regularized analogue of the kernel of the fermionic projector and the closed chain.

Definition 2.2.11 (Regularized Kernel of the Fermionic Projector)

Let $x, y \in \mathscr{M}$ be elements of physical spacetime and let S_x^ε and S_y^ε be the regularized spin spaces at $x \in \mathscr{M}$ and $y \in \mathscr{M}$, respectively. The *regularized kernel of the fermionic projector* is the mapping $P^\varepsilon(x,y) : S_y^\varepsilon \to S_x^\varepsilon$ defined as

$$u \mapsto \big[P^\varepsilon(x,y)\big](u) \overset{(2.13)}{:=} \big(\pi_{F^\varepsilon(x)} F^\varepsilon(y)|_{S_y^\varepsilon}\big)(u) \tag{2.18}$$

Definition 2.2.12 (Regularized Closed Chain)

Let $x, y \in \mathscr{M}$ be elements of physical spacetime and let S_x^ε be the regularized spin space at $x \in \mathscr{M}$. The *regularized closed chain* is the mapping $A^\varepsilon(x,y) : S_x^\varepsilon \to S_x^\varepsilon$ defined in terms the regularized kernel of the fermionic projector as

$$u \mapsto A^\varepsilon(x,y)(u) \overset{(2.18)}{:=} [P^\varepsilon(x,y) P^\varepsilon(y,x)](u) \tag{2.19}$$

As a consequence of the fact that both S_x^ε and S_y^ε are four-dimensional complex vector spaces and since $P^\varepsilon(x,y)$ is a bounded linear operator, we can regard it as an element $P^\varepsilon(x,y) \in \mathrm{L}(S_y^\varepsilon, S_x^\varepsilon)$. Although this definition is perfectly fine and natural in view of the definition of the kernel of the fermionic projector, we want to regard the regularized kernel of the fermionic projector as a section in a yet undetermined vector bundle over the base space $\mathscr{M} \times \mathscr{M}$. In order to implement this new point of view, we proceed as sketched in the following two paragraphs.

The Vector Bundle of Regularized Spin Spaces

As a first step towards a more geometric description we introduce the vector bundle $\pi : S^\varepsilon \to \mathscr{M}$ over the smooth Lorentzian manifold $(\mathscr{M}, g)$ where for each $x \in \mathscr{M}$ the corresponding fibre $\pi^{-1}(x)$ is given by the regularized spin space S_x^ε at $x \in \mathscr{M}$ which is a four-dimensional complex vector space.[11] In this setting, the regularized kernel of the fermionic projector $P^\varepsilon(x,y)$ can be regarded as a mapping between the fibres $\pi^{-1}(y)$ and $\pi^{-1}(x)$ of the vector bundle $\pi : S^\varepsilon \to \mathscr{M}$. To arrive at the desired description, however, this bundle is not sufficient. Instead, we have to go one step further and construct a vector bundle over the base space $\mathscr{M} \times \mathscr{M}$ as we now explain.

The Modified External Tensor Product Bundle

Having the smooth vector bundle $\pi : S^\varepsilon \to \mathscr{M}$ at our disposal, we take two copies and construct a new vector bundle over $\mathscr{M} \times \mathscr{M}$ in the following way:[12] First, we define for $i = 1, 2$ the projections $\mathrm{pr}_i : \mathscr{M} \times \mathscr{M} \to \mathscr{M}$ onto the i^{th} factor of the Cartesian product and subsequently introduce the pullback bundles $\tilde{\pi}_i : \mathrm{pr}_i^* S^\varepsilon \to \mathscr{M} \times \mathscr{M}$ with total spaces (again, for $i = 1, 2$) defined as

$$\mathrm{pr}_i^* S^\varepsilon \coloneqq \Big\{ ((z_1, z_2), \psi) \in (\mathscr{M} \times \mathscr{M}) \times S^\varepsilon \,\Big|\, \mathrm{pr}_i(z_1, z_2) = \pi_i(\psi) \Big\} \tag{2.20}$$

and projections given by $\tilde{\pi}_i(z_1, z_2, \psi) \coloneqq (z_1, z_2)$.[52, Def. 5.8] From these two pullback bundles which are defined over the same base space $\mathscr{M} \times \mathscr{M}$, we can now construct the sought-after vector bundle $\Pi : S^\varepsilon \boxtimes S^\varepsilon \to \mathscr{M} \times \mathscr{M}$ whose total space is defined as

$$S^\varepsilon \boxtimes S^\varepsilon \coloneqq \mathrm{Hom}(\mathrm{pr}_2^* S^\varepsilon, \mathrm{pr}_1^* S^\varepsilon) \tag{2.21}$$

and its fibres are given by $\Pi^{-1}\big((x_1, x_2)\big) = \mathrm{Hom}\big((\mathrm{pr}_2^* S^\varepsilon)_{(x_1,x_2)}, (\mathrm{pr}_1^* S^\varepsilon)_{(x_1,x_2)}\big)$.[13] By employing the definition of the pullback bundles, the fibres $\Pi^{-1}\big((x_1, x_2)\big)$ of this new vector bundle can be specified even more explicitly as the following calculation shows

$$\begin{aligned}
\tilde{\pi}_i^{-1}\big((x_1, x_2)\big) &= \big\{ ((z_1, z_2), \psi) \in (\mathscr{M} \times \mathscr{M}) \times S^\varepsilon \,\big|\, \mathrm{pr}_i(z_1, z_2) = \pi_i(\psi) \ \wedge\ \tilde{\pi}_i((z_1, z_2), \psi) = (x_1, x_2) \big\} \\
&= \big\{ ((z_1, z_2), \psi) \in (\mathscr{M} \times \mathscr{M}) \times S^\varepsilon \,\big|\, z_i = \pi_i(\psi) \ \wedge\ (z_1, z_2) = (x_1, x_2) \big\} \\
&= \begin{cases} \big\{ ((z_1, z_2), \psi) \in (\mathscr{M} \times \mathscr{M}) \times S^\varepsilon \,\big|\, (\pi_1(\psi), z_2) = (x_1, x_2) \big\} & \text{for } i = 1 \\ \big\{ ((z_1, z_2), \psi) \in (\mathscr{M} \times \mathscr{M}) \times S^\varepsilon \,\big|\, (z_1, \pi_2(\psi)) = (x_1, x_2) \big\} & \text{for } i = 2 \end{cases} \\
&= \begin{cases} S^\varepsilon_{x_1} \times \{x_2\} & \text{for } i = 1 \\ \{x_1\} \times S^\varepsilon_{x_2} & \text{for } i = 2 \end{cases}
\end{aligned} \tag{2.22}$$

Identifying $\tilde{\pi}_1^{-1}\big((x_1, x_2)\big) = S^\varepsilon_{x_1} \times \{x_2\}$ with $S^\varepsilon_{x_1}$ and analogously $\tilde{\pi}_2^{-1}\big((x_1, x_2)\big) = \{x_1\} \times S^\varepsilon_{x_2}$ with $S^\varepsilon_{x_2}$,[14] we arrive at the characterization of the fibres of the new bundle as

$$\Pi^{-1}\big((x_1, x_2)\big) \simeq \mathrm{Hom}\big(S^\varepsilon_{x_2}, S^\varepsilon_{x_1}\big) \tag{2.23}$$

By recalling that the regularized kernel of the fermionic projector as introduced in Definition 2.2.11 is an element $P^\varepsilon(x, y) \in \mathrm{L}(S^\varepsilon_y, S^\varepsilon_x) = \mathrm{Hom}(S^\varepsilon_y, S^\varepsilon_x)$, the above result allows to introduce a different, bundle-theoretic interpretation of the regularized kernel of the fermionic projector.

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[11] According to Lee's *Vector Bundle Chart Lemma*, the vector bundle $\pi : S^\varepsilon \to \mathscr{M}$ is actually a smooth vector bundle.[50, Lem. 10.6]

[12] Here we follow the construction as presented by Finster and Kraus.[51, Sec. 3]

[13] We remark that the non-standard notation has been deliberately chosen in order to both indicate the similarity with the so-called *external tensor product*, but at the same time to emphasize a slight difference: While the external tensor product of two vector bundles $\pi_1 : E_1 \to X_1$ and $\pi_2 : E_2 \to X_2$ is the vector bundle $E_1 \boxtimes E_2$ on $X_1 \times X_2$ with the total space given by $E_1 \boxtimes E_2 = \pi_1^* E_1 \otimes \pi_2^* E_2$, our bundle has its order reversed and includes an additional dualization.[53, Ch. 1, Sec. 4.9] Thus, in a sense, our bundle may be regarded as being "located halfway in between" the vector bundle of homomorphisms and the external tensor product.

[14] The bundle maps $\varphi_i : \mathrm{pr}_i^* S^\varepsilon \to S^\varepsilon$ from the pullback bundles $\mathrm{pr}_i^* S^\varepsilon$ to S^ε are given by $\varphi_i((x_1, x_2), \psi) = \psi$. Each fibre of the pullback bundle is homeomorphic to the fibre of the original bundle.

Definition 2.2.13 (Regularized Kernel of the Fermionic Projector (Section))

The *regularized kernel of the fermionic projector* is the section $\mathrm{P}^\varepsilon \in \Gamma(\mathscr{M} \times \mathscr{M}, S^\varepsilon \boxtimes S^\varepsilon)$ of the vector bundle $\Pi : S^\varepsilon \boxtimes S^\varepsilon \to \mathscr{M} \times \mathscr{M}$, which upon evaluation at $(x, y) \in \mathscr{M} \times \mathscr{M}$, reproduces $P^\varepsilon(x, y)$

$$\mathrm{P}^\varepsilon(x, y) := P^\varepsilon(x, y) \in \mathrm{Hom}(S^\varepsilon_y, S^\varepsilon_x) \tag{2.24}$$

where $P^\varepsilon(x, y)$ denotes the kernel of the fermionic projector as introduced in Definition 2.2.11.

We remark that the section P^ε cannot be chosen independently of the vector bundle $\Pi : S^\varepsilon \boxtimes S^\varepsilon \to \mathscr{M} \times \mathscr{M}$ as there is, by construction, an inextricable connection between both: Modifying the microstructure of physical spacetime corresponds to a different choice of the regularization operators $\mathfrak{R}^\varepsilon$ which in turn results in another local correlation function. But since the local correlation function enters both the definition of the vector bundles $\pi_i : S^\varepsilon \to \mathscr{M}$ as well as the definition of $P^\varepsilon(x, y)$ without altering its basic structure (see (2.18)), the section $\mathrm{P}^\varepsilon \in \Gamma(\mathscr{M} \times \mathscr{M}, S^\varepsilon \boxtimes S^\varepsilon)$ is essentially completely determined by the choice of the microstructure of physical spacetime.

2.2.4 The Regularized Causal Lagrangian and Action

Comparing the structure of the present chapter with the previous one reveals that we have changed the order in which objects are introduced. This is, of course, not accidental, but fully intentional: Due to the fact that the causal Lagrangian ultimately depends on the kernel of the fermionic projector via the closed chain and its eigenvalues, and furthermore taking into account that also the foundational conceptions are built into the kernel of the fermionic projector, it becomes clear that the regularized counterparts of the causal Lagrangian and the causal action are best regarded as functionals depending on the regularized kernel of the fermionic projector in order to analyze their dependence on the chosen regularization.

2.2.4.1 Classical Interpretation

The classical point of view is to regard the regularized objects as the "pullback" of the abstract objects by the local correlation function F^ε from the operator set $\mathcal{F}_n$ to physical spacetime $\mathscr{M}$. In this way, we obtain concrete realizations of the abstract objects which are defined on $\mathscr{M}$.

Definition 2.2.14 (Regularized Causal Lagrangian)

The *regularized causal Lagrangian* is the function $\mathcal{L}^\varepsilon : \mathscr{M} \times \mathscr{M} \to \mathbb{R}^+_0$ defined as

$$(x, y) \mapsto \mathcal{L}^\varepsilon(x, y) \overset{(1.7)}{\underset{(2.13)}{:=}} \mathcal{L}(\mathrm{F}^\varepsilon(x), \mathrm{F}^\varepsilon(y)) \tag{2.25}$$

where $\mathcal{L}$ and F^ε denote the causal Lagrangian and the local correlation function, respectively.

Based on this definition, the regularized causal action is defined as follows.

Definition 2.2.15 (Regularized Causal Action)

Let $(\mathcal{H}, \mathcal{F}_2, \rho^\varepsilon)$ be the causal fermion system constructed in Section 2.2 which models the physical vacuum system consisting of the Lorentzian manifold $(\mathscr{M}, g)$ without any particles or antiparticles present. The *regularized causal action* $\mathcal{S}^\varepsilon$ is defined as

$$\mathcal{S}^\varepsilon := \mathcal{S}(\rho^\varepsilon) \overset{(1.12)}{\underset{(2.15)}{=}} \iint\limits_{\mathcal{F}_2\times\mathcal{F}_2} \mathcal{L}(x,y)\, \mathrm{d}\rho^\varepsilon(x)\, \mathrm{d}\rho^\varepsilon(y) \tag{2.26}$$

By making use of the change-of-variable formula for pushforward measures[54, Thm. 3.6.1], the local correlation function contained in the regularized universal measure ρ^ε can be combined with the causal Lagrangian such that the regularized causal action can be expressed in terms of the regularized causal Lagrangian as

$$\mathcal{S}^\varepsilon \overset{(2.25)}{=} \iint\limits_{\mathscr{M}\times\mathscr{M}} \mathcal{L}^\varepsilon(x,y)\; \mathrm{d}\mu_g(x)\, \mathrm{d}\mu_g(y) \tag{2.27}$$

Especially in the second form it becomes apparent that the regularized causal action, for a given physical spacetime $(\mathscr{M}, g)$, is basically a functional of the chosen regularization. In order to clarify how $\mathcal{S}^\varepsilon$ depends on the regularization and, as a consequence, how it changes due to variations of the regularization, the following alternative point of view is beneficial.

2.2.4.2 Bundle-Theoretic Description

While in the classical interpretation the regularized causal Lagrangian is considered as a real-valued function on physical spacetime which is obtained by combing the causal Lagrangian with the local correlation function, an alternative point of view is to regard the regularized causal Lagrangian as a functional of sections of the vector bundle $\Pi : S^\varepsilon \boxtimes S^\varepsilon \to \mathscr{M}\times\mathscr{M}$ introduced above.

Definition 2.2.16 (Causal Lagrangian Evaluation Operator)

The *causal Lagrangian evaluation operator* is defined as the mapping $\Lambda : \Gamma(\mathscr{M}\times\mathscr{M}, S^\varepsilon \boxtimes S^\varepsilon) \to C^\infty(\mathscr{M}\times\mathscr{M}, \mathbb{R}_0^+)$ which to a regularized kernel of the fermionic projector P^ε associates the regularized causal Lagrangian

$$\Lambda : \mathrm{P}^\varepsilon \mapsto \Lambda[\mathrm{P}^\varepsilon] := \mathcal{L}^\varepsilon \tag{2.28}$$

This causal Lagrangian evaluation operator establishes the connection between the foundational conceptions underlying the whole modelling approach (and, in particular, the microstructure of physical spacetime $\mathscr{M}$ abstractly encoded in P^ε) and the causal relation between all possible pairs $(x,y) \in \mathscr{M}\times\mathscr{M}$ of points in physical spacetime.[15] Continuing this line of thought, one is directly led to introduce also the corresponding evaluation operator for the regularized causal action.

Definition 2.2.17 (Causal Action Evaluation Operator)

The *causal action evaluation operator* is the mapping $\Sigma : \Gamma(\mathscr{M}\times\mathscr{M}, S^\varepsilon \boxtimes S^\varepsilon) \to \mathbb{R}_0^+$ which to a given regularized kernel of the fermionic projector P^ε associates the regularized causal action $\mathcal{S}^\varepsilon$

$$\Sigma : \mathrm{P}^\varepsilon \mapsto \Sigma[\mathrm{P}^\varepsilon] := \mathcal{S}^\varepsilon \overset{(2.27)}{\underset{(2.28)}{=}} \iint\limits_{\mathscr{M}\times\mathscr{M}} \big(\Lambda[\mathrm{P}^\varepsilon]\big)(x,y)\; \mathrm{d}\mu_g(x)\, \mathrm{d}\mu_g(y) \tag{2.29}$$

where the regularized causal Lagrangian $\mathcal{L}^\varepsilon(x,y)$ at $(x,y) \in \mathscr{M}\times\mathscr{M}$ has been replaced by the causal Lagrangian evaluation operator $\Lambda[\mathrm{P}^\varepsilon]$ evaluated at $(x,y) \in \mathscr{M}\times\mathscr{M}$.

[15] We remark that this point of view resembles the presentation in the earlier days of the theory where the causal Lagrangian was regarded as a "real-valued functional on the endomorphisms of $S_x \subset \mathcal{H}_\mathbb{C}$".[6, Sec. 3.5] Here we go one step further and regard the (regularized) Lagrangian basically as a functional of the (regularized) kernel of the fermionic projector instead of the (regularized) closed chain.

This alternative perspective will be the starting point for the derivation of variations of the regularized causal action in Chapter 3 as it allows both for a more intuitive understanding as well as a more direct relation between deformations of the regularization leading to a modified regularized kernel of the fermionic projector and the resulting variations of the regularized causal action. For a schematic graphical representation we refer to Figure 2.1.

2.3 Special Case: Modelling the Minkowski Vacuum

Now that we have explained how physical vacuum systems can be modelled within the theory of causal fermion systems which hopefully will be of some use to future doctoral students as a brief summary and complementation of the already existing literature, we conclude this chapter by narrowing down our field of view to the case where the physical vacuum system is given by Minkowski spacetime without any particles or antiparticles present which is usually referred to as the *Minkowski vacuum*. This restriction has far-reaching consequences as it leads to a number of simplifications and in this way makes it possible to perform explicit calculations in the following chapters of Part II and Part III.

2.3.1 Construction of the iε-Regularized Causal Fermion System

Without intending to repeat the entire construction procedure for a causal fermion system $(\mathcal{H}, \mathcal{F}_2, \rho^\varepsilon)$ as presented in Subsection 2.2.1 and Subsection 2.2.2, we merely want to point out where the choice of Minkowski space as physical spacetime in the physical vacuum system affects the construction and how this modification leads to considerable simplifications.[16]

The Hilbert Space of Negative-Frequency Dirac Solutions

In Subsection 2.2.1 we have seen that the crucial step to implement Assumption 2.2.1 in general Lorentzian manifolds $(\mathscr{M}, g)$ was the insight that we need to impose global hyperbolicity of the time-oriented Lorentzian manifold in order to ensure that the Cauchy problem for the Dirac equation is well-posed. Due to the fact that Minkowski space $(\mathscr{M}, \eta)$ satisfies both the strong causality condition as well as the compactness condition for causal diamonds, it is globally hyperbolic and thus allows to find a unique global solution $\psi \in \Gamma^\infty_{\text{sc}}(\mathscr{N}_t, S\mathscr{M})$ of the Dirac equation with compact support on any other Cauchy hypersurface $\mathscr{N}_t$ for compactly-supported initial data $\psi_0 \in \Gamma^\infty_{\text{sc}}(\mathscr{N}_{t_0}, S\mathscr{M})$ on a Cauchy hypersurface $\mathscr{N}_{t_0}$. Furthermore, we can choose the trivial spin connection and thus identify the spinor spaces $S_x\mathscr{M}$ at different physical spacetime points $x \in \mathscr{M}$ with $\mathbb{C}^4$ such that the spinor bundle becomes the trivial vector bundle $S\mathscr{M} = \mathscr{M} \times \mathbb{C}^4$. Along with all this, the Dirac equation reduces to $(\mathrm{i}\gamma^j \partial_j - m)\psi = 0$ and correspondingly also the inner product (2.4) on solutions boils down to

$$(\psi|\phi)_m := 2\pi \int_{\mathbb{R}^3} \mathrm{d}\mu_{\mathbb{R}^3}(\vec{x}) \; \prec\psi|\gamma^0\phi\succ_{S_x\mathscr{M}} \tag{2.30}$$

where we have chosen the future-directed normal ν as $\nu_j = \delta_{j0}$ which corresponds to Cauchy hypersurfaces $\mathscr{N}_t = \{(t, \vec{x}) \in \mathscr{M} \mid t = \text{const}\} \simeq \mathbb{R}^3$. Just as before, the measure on the Cauchy hypersurface is the Lebesgue-Borel measure corresponding to the Riemannian volume form which, in turn, is induced by the Lorentzian volume form. Making use of the fact that solutions of the Dirac equation in this setting are given by plane waves[55, Sec. 1.4]

$$\psi_{\vec{p}a\pm}(x) = \frac{1}{\sqrt{(2\pi)^3}} \chi_{\vec{p}a\pm} \mathrm{e}^{-\mathrm{i}(\pm\omega_p)x^0 + \mathrm{i}\vec{p}\cdot\vec{x}} \qquad \text{with} \qquad \omega_p := \sqrt{|\vec{p}|^2 + m^2} \tag{2.31}$$

[16] This subsection basically follows the presentation in the introductory article by Finster and Jokel[26, Sec. 4.3], but in part also relies on the work by Finster and Grotz.[22, Sec. 4.1].

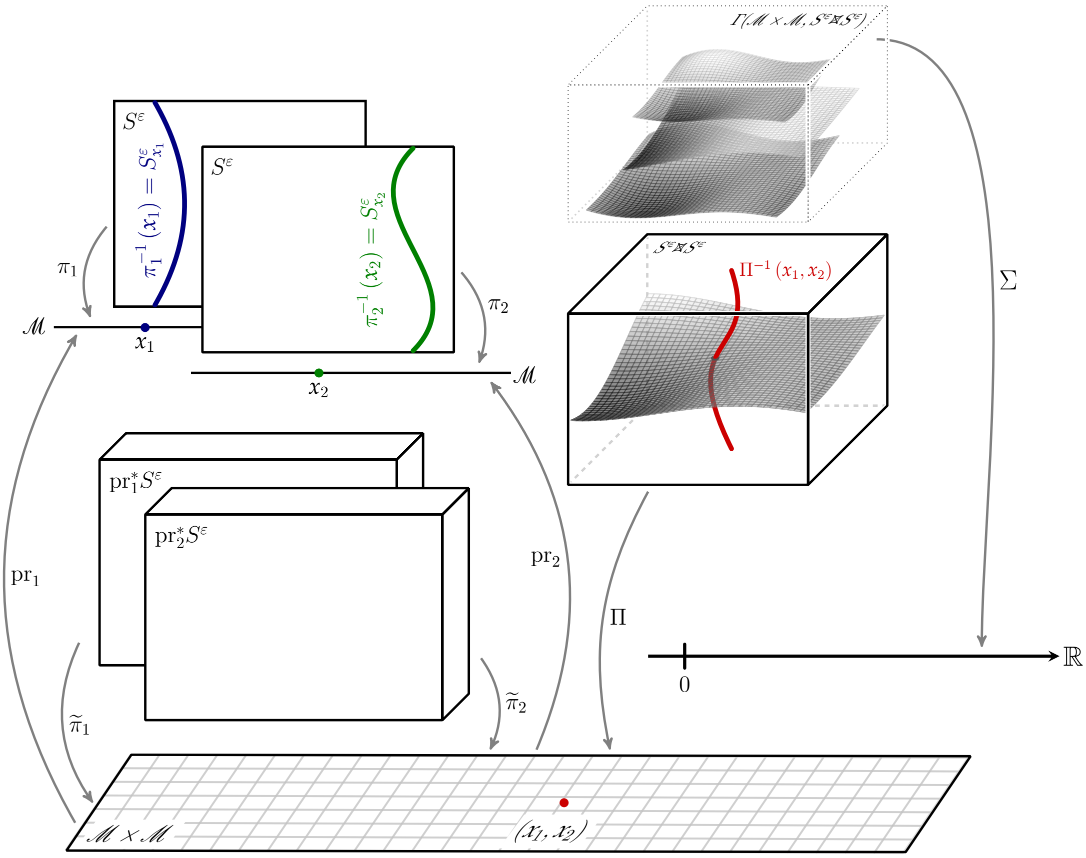


Figure 2.1: Schematic graphical representation of the relation between the vector bundles $\pi_i : S^\varepsilon \to \mathscr{M}$, the pullback bundles $\tilde{\pi}_i : \mathrm{pr}_i^* S^\varepsilon \to \mathscr{M} \times \mathscr{M}$ and the new vector bundle $\Pi : S^\varepsilon \boxtimes S^\varepsilon \to \mathscr{M} \times \mathscr{M}$ as well as the causal action evaluation operator $\Sigma : \Gamma(\mathscr{M} \times \mathscr{M}, S^\varepsilon \boxtimes S^\varepsilon) \to \mathbb{R}_0^+$.

where the spinor $\chi_{\vec{p}a\pm} \in \mathbb{C}^4$ solves the algebraic equation $(\gamma^j p_j - m)\chi_{\vec{p}a\pm} = 0$, we can form so-called *negative-frequency wave-packets*

$$\psi_f(x) := \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ f(\vec{p})\psi_{\vec{p}a-}(x) \qquad \text{with} \qquad f \in C_0^\infty(\mathbb{R}^3, \mathbb{C}) \tag{2.32}$$

and thus realize the Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle_\mathcal{H})$ of negative-frequency solutions of the Dirac equation as

$$\mathcal{H} := \overline{\left\{\psi_f \in C_0^\infty(\mathscr{M}, \mathbb{C}^4) \,\middle|\, (\mathrm{i}\gamma^j\partial_j - m)\psi_f = 0\right\}}^{(\cdot|\cdot)_m} \tag{2.33}$$

without the necessity to first construct the Hilbert space $(\mathcal{H}_m, (\cdot|\cdot)_m)$ of all solutions of the Dirac equation and only afterwards choose the closed subspace $(\mathcal{H}, \langle\cdot|\cdot\rangle_\mathcal{H})$ corresponding to the Dirac sea.

The Set of Operators and the Regularized Universal Measure

With the Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle_\mathcal{H})$ corresponding to the negative-frequency solutions of the Dirac equation at hand, we next have to specify the set of operators and the regularized universal measure by constructing the local correlation function in the same way as described in Subsection 2.2.2.1. To this end, we first of all have to specify how the regularization operators, which according to Section 2.1 reflects a certain geometric idea regarding the microstructure of physical spacetime, should be chosen. Due to the fact that the regularization is built into the regularized causal Lagrangian in a rather complicated way, the complexity of the intended microstructure of physical spacetime must be weighed against the technical manageability of its implementation. As it turns out, however, even rudimentarily realistic regularizations such as the setting where the regularization operators are given by convolution operators, leads to an considerable technical effort.[17] For this reason the easily manageable, so-called iε*-regularization* is used almost without exception in the literature. Taking the negative-frequency wave-packets as the starting point, the regularization operators are thus defined as[26, Sec. 4.2]

$$(\mathfrak{R}^\varepsilon \psi_f)(x) := \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ f(\vec{p})\psi_{\vec{p}a-}(x)\mathrm{e}^{-\varepsilon\omega_p} \tag{2.34}$$

where the additional exponential factor leads to an ε-dependent suppression of high-frequency contributions.[18] By inserting this result into Definition 2.2.6 (Local Correlation Function) it can be shown[22, Prop. 4.1] that for any $x \in \mathscr{M}$ the local correlation operator $\mathrm{F}^\varepsilon(x)$ has two positive and two negative eigenvalues and thus leads, together with the associated regularized universal measure ρ^ε, to a causal fermion system $(\mathcal{H}, \mathcal{F}_2, \rho^\varepsilon)$ of spin dimension $n = 2$ which corresponds to the Dirac sea vacuum in Minkowski spacetime.

2.3.2 The iε-Regularized Kernel of the Fermionic Projector

The simplifications accompanying the specialization to Minkowski spacetime allow to regard the regularized kernel of the fermionic projector as a function $\mathrm{P}^\varepsilon \in C^\infty(\mathscr{M} \times \mathscr{M}, \mathrm{L}(\mathbb{C}^4, \mathbb{C}^4))$ rather than a section in a vector bundle.[19] Although the iε-regularized kernel of the fermionic projector will not enter the stage before Part III, we nevertheless shall introduce it already at this point for the sake of completeness. Taking the local correlation function as the starting point, it can be shown that the iε-regularized kernel of the fermionic projector takes the following form, which we state as a definition at this point.[20]

Definition 2.3.1 (iε-Regularized Kernel of the Fermionic Projector)

Let $(\mathscr{M}, \eta)$ be Minkowski spacetime and let $\varepsilon > 0$. For any two physical spacetime points $x, y \in \mathscr{M}$, the iε-regularized kernel of the fermionic projector $\mathrm{P}^\varepsilon \in C^\infty(\mathscr{M} \times \mathscr{M}, \mathrm{L}(\mathbb{C}^4, \mathbb{C}^4))$ is the function which, upon evaluation at $(x, y) \in \mathscr{M} \times \mathscr{M}$, is given by

$$(x, y) \mapsto \mathrm{P}^\varepsilon(x, y) := \int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\ (\not{p} + \mu\, \mathrm{id}_{\mathbb{C}^4})\delta(p^2 - \mu^2)\Theta(-p^0)\mathrm{e}^{-\mathrm{i}p(x-y)}\mathrm{e}^{-\varepsilon|p^0|} \tag{2.35}$$

where $\not{p} := \gamma^j p_j$ denotes the Feynman slash and $p^2 := \eta(p, p)$ as well as $p(x - y) := \eta(p, x - y)$ are shorthand notations for the Minkowski space inner product. Note that in view of the fact that m will be needed as one of the multipole parameters later on, we from now on denote the mass parameter in the Dirac equation by μ.

One of the special properties of this iε-regularized kernel of the fermionic projector is its dependence on the difference vector $\xi := y - x$ which reflects invariance of Minkowski spacetime under translations. This property of regularized kernels of the fermionic projectors is referred to as *homogeneity* and is one of the foundational assumptions on the class of regularized kernels of the fermionic projector which will be studied in the following Chapter 3. As will turn out below, the following definition allows for a more compact notation.

[17] We point out that this must not be misunderstood as weakness of whole theory, but merely as a manifestation of the yet unknown answer to the question how physical spacetime looks on microscopic length scales: In order not to exclude certain microstructures right from the start, one has to accept a large degree of complexity.

[18] The terminology iε-regularization stems from the fact that combining the additional exponential factor with the plane-wave factor contained in $\psi_{\vec{p}q-}(x)$ leads to the appearance of the factor $(x^0 + \mathrm{i}\varepsilon)$ in the exponential which may be understood as resulting from the replacement $x^0 \to x^0 + \mathrm{i}\varepsilon$.[11, Sec. 2.4.1]

[19] Note that the regularized kernel of the fermionic projector, in particular in the context of (regularized) Hadamard states[56], is usually referred to as a tempered *bi-distribution* on $\mathscr{M} \times \mathscr{M}$.[46, Thm. 3.12]

[20] The derivation of the iε-regularized kernel of the fermionic projector starting from (2.34) has been explained by Finster and Grotz[22, Sec. 4.1] in such captivating clarity that we could not add anything of value to it and thus shall directly refer to the corresponding section.

Definition 2.3.2 (Regularized Difference Vector)

The *regularized difference vector* $\xi^\varepsilon_\mp$ is defined as $\xi^\varepsilon_\mp = (\xi^0 \mp \mathrm{i}\varepsilon, \vec{\xi})$ where $\xi := y - x$. Additionally, the *dimensionless regularized variable* $\Xi^\varepsilon_\mp$ is the function $\Xi^\varepsilon_\mp : \mathbb{R} \times \mathbb{R}^+_0 \to \mathbb{C}$ defined as

$$(\xi^0, r) \mapsto \Xi^\varepsilon_\mp(\xi^0, r) := \mu\sqrt{-(\xi^\varepsilon_\mp)^2} \tag{2.36}$$

where $\mu \in \mathbb{R}^+_0$ is the mass appearing in (2.35) and $r := |\vec{\xi}|$.

After these preparatory considerations, we now derive an explicit expression for the iε-regularized kernel of the fermionic projector by evaluating the Fourier integral in its definition.

Lemma 2.3.3 (iε-Regularized Kernel of the Fermionic Projector)

The Fourier integral in the definition of the iε-regularized kernel of the fermionic projector evaluates to

$$\mathrm{P}^\varepsilon(x, y) = \sum_{j=0}^{3} g^\varepsilon_-(\xi)(\xi^\varepsilon_-)_j \gamma^j + h^\varepsilon_-(\xi)\mathrm{id}_{\mathbb{C}^4} \tag{2.37}$$

where the functions $g^\varepsilon_-, h^\varepsilon_- \in C^\infty(\mathbb{R}^4, \mathbb{C})$, expressed in terms of modified Bessel functions of the second kind and the dimensionless regularized variable Ξ^ε_-, are given by

$$g^\varepsilon_-(\xi) = -\mathrm{i}\frac{\mu^4}{(2\pi)^3}\frac{K_2(\Xi^\varepsilon_-)}{(\Xi^\varepsilon_-)^2} \tag{2.37a}$$

$$h^\varepsilon_-(\xi) = \frac{\mu^3}{(2\pi)^3}\frac{K_1(\Xi^\varepsilon_-)}{\Xi^\varepsilon_-} \tag{2.37b}$$

Here and in what follows we always identify $\{\xi := y - x \,|\, x, y \in \mathscr{M}\} \simeq \mathbb{R}^4$.

Proof. To evaluate the Fourier integral (2.35) we first rewrite the factor $(\not{p} + \mu\,\mathrm{id}_{\mathbb{C}^4})\mathrm{e}^{-\mathrm{i}p(x-y)}$ as a derivative of the exponential factor with respect to ξ as

$$(\not{p} + \mu\,\mathrm{id}_{\mathbb{C}^4})\mathrm{e}^{-\mathrm{i}p(x-y)} = (p_j\gamma^j + \mu\,\mathrm{id}_{\mathbb{C}^4})\mathrm{e}^{+\mathrm{i}p\xi} = \left(-\mathrm{i}\gamma^j\frac{\partial}{\partial\xi^j} + \mu\,\mathrm{id}_{\mathbb{C}^4}\right)\mathrm{e}^{\mathrm{i}p\xi}$$

Furthermore, by employing the distributional relation

$$\delta(p^2 - \mu^2) = \delta\big((p^0)^2 - (|\vec{p}|^2 + \mu^2)\big) \overset{(2.31)}{=} \frac{\delta(p^0 - \omega_p) + \delta(p^0 + \omega_p)}{2\omega_p}$$

where we used the definition $\omega_p = \sqrt{|\vec{p}|^2 + \mu^2}$ introduced in (2.31), we find

$$\begin{aligned}\mathrm{P}^\varepsilon(x, y) &\overset{(2.35)}{=} \left(-\mathrm{i}\gamma^j\frac{\partial}{\partial\xi^j} + \mu\,\mathrm{id}_{\mathbb{C}^4}\right)\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\vec{p}}{(2\pi)^4}\int_{-\infty}^{0}\mathrm{d}p^0\,\frac{\delta(p^0 - \omega_p) + \delta(p^0 + \omega_p)}{2\omega_p}\mathrm{e}^{\mathrm{i}p\xi^\varepsilon_-}\\ &= \left(-\mathrm{i}\gamma^j\frac{\partial}{\partial\xi^j} + \mu\,\mathrm{id}_{\mathbb{C}^4}\right)\int_{\mathbb{R}^4}\frac{\mathrm{d}^3\vec{p}}{(2\pi)^4}\,\frac{\mathrm{e}^{-\mathrm{i}\omega_p(\xi^\varepsilon_-)^0}}{2\omega_p}\mathrm{e}^{\mathrm{i}\vec{p}\cdot\vec{\xi}}\end{aligned}$$

Choosing a spherical coordinate system with its polar axis pointing in the direction of $\vec{\xi}$, carrying out the angular integrals and expressing everything in terms of trigonometric functions results in

$$\ldots = \left(-\mathrm{i}\gamma^j\frac{\partial}{\partial\xi^j} + \mu\,\mathrm{id}_{\mathbb{C}^4}\right)\int_0^\infty\frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}\,\frac{\mathrm{e}^{-\mathrm{i}\omega_p(\xi^\varepsilon_-)^0}}{\omega_p}\,\frac{\sin(|\vec{p}|r)}{|\vec{p}|r}$$

To compute the remaining integral we interpret it as a Fourier sine transform, identify $\alpha \equiv r$, $\beta \equiv \mathrm{i}(\xi^0 - \mathrm{i}\varepsilon) \equiv \varepsilon + \mathrm{i}\xi^0$ and $\gamma = \mu$ evaluate it using (A.1b) such that we end up with

$$\ldots \overset{\text{(A.1b)}}{=} \left(-\mathrm{i}\gamma^j \frac{\partial}{\partial \xi^j} + \mu\, \mathrm{id}_{\mathbb{C}^4} \right) \frac{\mu}{(2\pi)^3} \frac{K_1(\mu\sqrt{r^2 + (\varepsilon + \mathrm{i}\xi^0)^2})}{\sqrt{r^2 + (\varepsilon + \mathrm{i}\xi^0)^2}} \tag{2.38}$$

Finally, by carrying out the derivatives[57, pp. 8.486/12] and expressing everything in terms of the regularized difference vector ξ_-^ε, we end up with

$$\begin{aligned} \mathrm{P}^\varepsilon(x,y) &= -\mathrm{i}\frac{\mu^4}{(2\pi)^3}\left(\frac{K_0(\Xi_-^\varepsilon)}{(\Xi_-^\varepsilon)^2} + 2\frac{K_1(\Xi_-^\varepsilon)}{(\Xi_-^\varepsilon)^3}\right)(\xi_-^\varepsilon)_j\gamma^j + \frac{\mu^3}{(2\pi)^3}\frac{K_1(\Xi_-^\varepsilon)}{\Xi_-^\varepsilon}\mathrm{id}_{\mathbb{C}^4} \\ &= -\mathrm{i}\frac{\mu^4}{(2\pi)^3}\frac{K_2(\Xi_-^\varepsilon)}{(\Xi_-^\varepsilon)^2}(\xi_-^\varepsilon)_j\gamma^j + \frac{\mu^3}{(2\pi)^3}\frac{K_1(\Xi_-^\varepsilon)}{\Xi_-^\varepsilon}\mathrm{id}_{\mathbb{C}^4} \end{aligned} \tag{2.39}$$

where we have used the recursion relation $K_2(z) = K_0(z) + 2z^{-1}K_1(z)$[57, 8.486/17] in the last step.

This concludes the proof. □

Remark 2.3.4 (Adjoint of iε-Regularized Kernel of the Fermionic Projector)

The adjoint $\mathrm{P}^\varepsilon(x,y)^*$ of the iε-regularized kernel of the fermionic projector can be expressed as $\mathrm{P}^\varepsilon(y,x)$ via the regularized analogue of Proposition 1.4.3. Taking homogeneity into account, we thus find

$$\mathrm{P}^\varepsilon(y,x) = \sum_{j=0}^{3} g_+^\varepsilon(\xi)(\xi_+^\varepsilon)_j\gamma^j + h_+^\varepsilon(\xi)\mathrm{id}_{\mathbb{C}^4} \tag{2.40}$$

where the functions $g_+^\varepsilon, h_+^\varepsilon \in C^\infty(\mathbb{R}^4, \mathbb{C})$ are given by

$$g_+^\varepsilon(\xi) = +\mathrm{i}\frac{\mu^4}{(2\pi)^3}\frac{K_2(\Xi_+^\varepsilon)}{(\Xi_+^\varepsilon)^2} \tag{2.40a}$$

$$h_+^\varepsilon(\xi) = \frac{\mu^3}{(2\pi)^3}\frac{K_1(\Xi_+^\varepsilon)}{\Xi_+^\varepsilon} \tag{2.40b}$$

2.3.3 The Homogeneous Regularized Causal Action

For a regularized kernel of the fermionic projector which is homogeneous, the corresponding regularized causal Lagrangian inherits this property via the eigenvalues of the regularized closed chain and thus also depends only on the difference vector $\xi := y - x$. As a consequence, one can change variables $(x,y) \to (x,\xi)$ in the double integral in Definition 2.2.15 (Regularized Causal Action) and first integrate with respect to the relative variable ξ and only afterwards carry out the integral with respect to x. The latter integration, however, gives a multiplicative infinite constant which turns $\mathcal{S}^\varepsilon$ into a divergent expression and thus suggests to introduce the following definition.[11, Sec. 4.2.2]

Definition 2.3.5 (Homogeneous Regularized Lagrangian and Causal Action)

Let $(\mathcal{H}, \mathcal{F}_2, \rho^\varepsilon)$ be a causal fermion system describing Minkowski spacetime $(\mathscr{M}, \eta)$ with a regularization chosen such that the regularized kernel of the fermionic projector is homogeneous. Then the *homogeneous regularized causal action* $\mathcal{S}_\mathrm{h}^\varepsilon$ is defined, by analogy with Definition 2.2.15, as[7, Eq. (4.5)]

$$\mathcal{S}_{\mathrm{h}}^{\varepsilon} := \int_{\mathbb{R}^4} \mathcal{L}_{\mathrm{h}}^{\varepsilon}(\xi)\ \mathrm{d}^4\xi \tag{2.41}$$

where $\mathcal{L}_{\mathrm{h}}^{\varepsilon} : \mathbb{R}^4 \to \mathbb{R}_0^+$ is referred to as the *homogeneous regularized causal Lagrangian.*

For the sake of completeness we remark that a conceptually more thorough way to introduce homogeneity is to consider symmetries of causal fermion systems[58, 59] and represent the (regularized) kernel of the fermionic projector in the homogeneous case using so-called *operator-valued negative-definite measures*[7, Def. 4.1] in a form which generalizes, but very much resembles the Fourier decomposition in Definition 2.3.1.[21]

Notation 2.3.6 (Homogeneous Regularized Lagrangian and Causal Action)

Whenever there is no risk of confusion, we will drop the subscripts indicating homogeneity and distinguish between the homogeneous and general setting only through the arguments.

2.3.4 The iε-Regularized Causal Lagrangian

To conclude this chapter, we want to discuss the iε-regularized causal Lagrangian in greater detail in order to develop a sense of how the iε-regularization affects the causal relation among difference vectors of physical spacetime points. To this end, we anticipate a result from Chapter 3, namely the expression for the regularized causal Lagrangian in terms of the components a regularized kernel of the fermionic projector with vector-scalar structure as derived in Lemma 3.4.1.

Lemma 2.3.7 (iε-Regularized Causal Lagrangian)

Let $(\mathscr{M}, \eta)$ be Minkowski space. Then, by anticipating the result from Lemma 3.4.1, the iε-regularized causal Lagrangian $\mathcal{L}_{\mathrm{h}}^{\varepsilon} : \mathbb{R}^4 \to \mathbb{R}_0^+$ evaluates to

$$\begin{aligned}\mathcal{L}_{\mathrm{h}}^{\varepsilon}(\xi) = 4\left(\frac{\mu}{2\pi}\right)^{12}\Bigg[&\mu^4\left(\left(|\xi^\varepsilon|^2\right)^2 - \left|(\xi_+^\varepsilon)^2\right|^2\right)\left|\frac{K_2(\Xi_-^\varepsilon)}{(\Xi_-^\varepsilon)^2}\right|^4 \\ &+ 2\mu^2\,\mathrm{Re}\left[|\xi^\varepsilon|^2\left|\frac{K_2(\Xi_-^\varepsilon)}{(\Xi_-^\varepsilon)^2}\,\frac{K_1(\Xi_-^\varepsilon)}{\Xi_-^\varepsilon}\right|^2 - (\xi_-^\varepsilon)^2\left(\frac{K_2(\Xi_-^\varepsilon)}{(\Xi_-^\varepsilon)^2}\,\frac{K_1(\Xi_+^\varepsilon)}{\Xi_+^\varepsilon}\right)^2\right]\Bigg]\end{aligned} \tag{2.42}$$

and has length dimension $\mathrm{ldim}(\mathcal{L}_{\mathrm{h}}^{\varepsilon}) = -12$.

Proof. To determine the explicit form of the regularized causal Lagrangian corresponding to the iε-regularized kernel of the fermionic projector introduced in Definition 2.3.1, we exploit its *vector-scalar structure* which allows to compute the iε-regularized causal Lagrangian via Lemma 3.4.1 as follows

$$\begin{aligned}\mathcal{L}^\varepsilon(x,y) &\overset{(2.25)}{\underset{(3.14)}{=}} 4\left[(B^\varepsilon(x,y))^2 - |C^\varepsilon(x,y)|^2\right] \\ &\overset{(3.15)}{=} 4\left[\left(|v^\varepsilon|^2(x,y) + |s^\varepsilon|^2(x,y)\right)^2 - \left|(\overline{v^\varepsilon})^2(x,y) - (\overline{s^\varepsilon})^2(x,y)\right|^2\right]\end{aligned} \tag{2.43}$$

Identifying $v_j^\varepsilon(x,y) \equiv g_-^\varepsilon(\xi)(\xi_-^\varepsilon)_j$, $s^\varepsilon(x,y) \equiv h_-^\varepsilon(\xi)$, $\overline{v_j^\varepsilon}(x,y) \equiv g_+^\varepsilon(\xi)(\xi_+^\varepsilon)_j$ and $\overline{s^\varepsilon}(x,y) \equiv h_+^\varepsilon(\xi)$

[21] This idea was outlined by Christoph Langer in a seminar talk on *Homogeneous Causal Fermion Systems*, but to the best of my knowledge, has not been published yet.

together with $|\xi^\varepsilon|^2 := \eta(\xi^\varepsilon_-, \xi^\varepsilon_+)$ and $(\xi^\varepsilon_\mp)^2 := \eta(\xi^\varepsilon_\mp, \xi^\varepsilon_\mp)$ results in

$$\begin{aligned}
\mathcal{L}^\varepsilon_{\mathrm{h}}(\xi) &= 4\Big[\big(|\xi^\varepsilon|^2|g^\varepsilon(\xi)|^2 + |h^\varepsilon(\xi)|^2\big)^2 - \big|(\xi^\varepsilon_+)^2 g^\varepsilon_+(\xi)^2 - h^\varepsilon_+(\xi)^2\big|^2\Big] \\
&= 4\Big[\Big(|\xi^\varepsilon|^2|\xi^\varepsilon|^2 - (\xi^\varepsilon_-)^2(\xi^\varepsilon_+)^2\Big)(|g^\varepsilon_-|^2)^2 + 2|\xi^\varepsilon|^2|g^\varepsilon_-|^2|h^\varepsilon_-|^2 + 2\,\mathrm{Re}\,\Big((\xi^\varepsilon_+)^2(g^\varepsilon_+)^2(h^\varepsilon_-)^2\Big)\Big] \\
&= 4\left(\frac{\mu}{2\pi}\right)^{12}\Bigg[\mu^4\Big(|\xi^\varepsilon|^2|\xi^\varepsilon|^2 - (\xi^\varepsilon_-)^2(\xi^\varepsilon_+)^2\Big)\left|\frac{K_2(\Xi^\varepsilon_-)}{(\Xi^\varepsilon_-)^2}\right|^4 \\
&\qquad + 2\mu^2|\xi^\varepsilon|^2\left|\frac{K_2(\Xi^\varepsilon_-)}{(\Xi^\varepsilon_-)^2}\frac{K_1(\Xi^\varepsilon_-)}{\Xi^\varepsilon_-}\right|^2 - 2\mu^2\,\mathrm{Re}\left[(\xi^\varepsilon_-)^2\left(\frac{K_2(\Xi^\varepsilon_-)}{(\Xi^\varepsilon_-)^2}\frac{K_1(\Xi^\varepsilon_+)}{\Xi^\varepsilon_+}\right)^2\right]\Bigg]
\end{aligned}$$

Taking into account that ξ^ε, μ and $\Xi^\varepsilon_\mp$ have length dimensions $+1$, -1 and 0, respectively, we conclude that the regularized causal Lagrangian has length dimension $\mathrm{ldim}(\mathcal{L}^\varepsilon_{\mathrm{h}}) = -12$.

This concludes the proof. □

Now, in order to study the causal relation among physical spacetime points $x, y \in \mathscr{M}$ in the homogeneous case, we are free to fix $x \in \mathscr{M}$ and analyze all physical spacetime points $y \in \mathscr{M}$ with respect to x. In this way, spacelike-separatedness of $x, y \in \mathscr{M}$ translates into $\mathcal{L}^\varepsilon_{\mathrm{h}}(\xi) = 0$ and thus suggests to introduce the following definition.

Definition 2.3.8 (Demarcation Function)

Let $\mathcal{L}^\varepsilon_{\mathrm{h}} : \mathbb{R}^4 \to \mathbb{R}^+_0$ be a homogeneous regularized causal Lagrangian. The *region* $\mathcal{R}^\varepsilon$ *of non-spacelike-separated difference vectors* is defined as

$$\mathcal{R}^\varepsilon := \big\{\xi \in \mathbb{R}^4 \,\big|\, \mathcal{L}^\varepsilon_{\mathrm{h}}(\xi) > 0\big\} \tag{2.44}$$

If $\mathcal{R}^\varepsilon$ satisfies the conditions stated in Assumption 3.2.3, the function $R^\varepsilon_{\max} : \mathbb{R} \times (0, \pi) \times (0, 2\pi) \to \mathbb{R}^+_0$ implicitly defined by[a]

$$\mathcal{L}^\varepsilon_{\mathrm{h}}(\xi^0, R^\varepsilon_{\max}(\xi^0, \theta, \varphi), \theta, \varphi) = 0 \tag{2.45}$$

is referred to as *demarcation function* as it marks the border between spacelike-separated difference vectors $\xi \in \mathbb{R}^4$ and non-spacelike-separated ones. In the special case when $R^\varepsilon_{\max}$ has no angular dependence, we often write

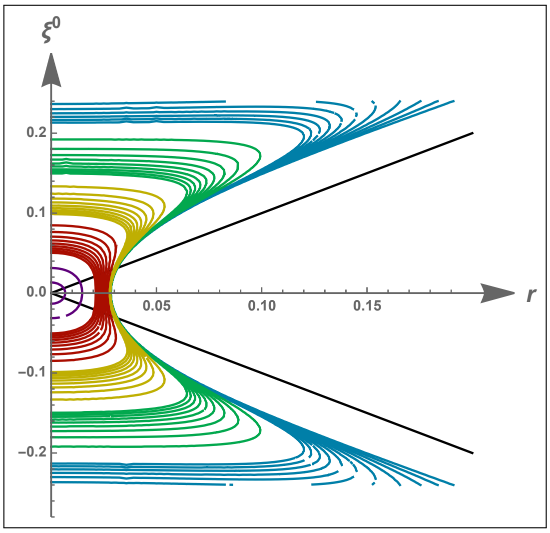
$$\mathcal{R}^\varepsilon = \mathcal{X}^\varepsilon \times S^2 \qquad \text{with} \qquad \mathcal{X}^\varepsilon := \{(\xi^0, r) \in \mathbb{R} \times \mathbb{R}^+_0 \,|\, 0 \le r \le R^\varepsilon_{\max}(\xi^0)\} \tag{2.46}$$

[a] If not otherwise stated, we will always work with spherical coordinates.

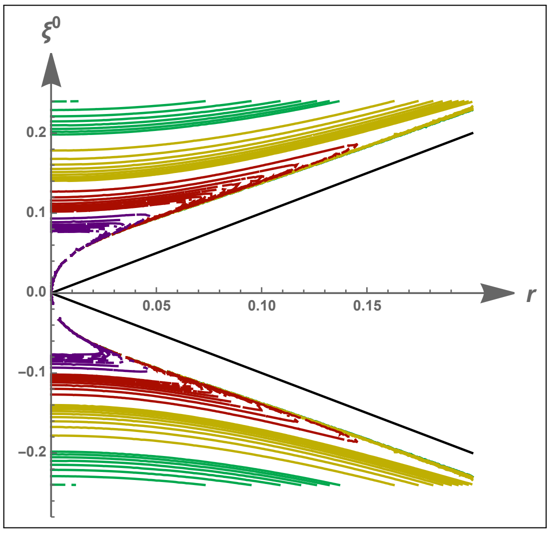
Due to the fact that the iε-regularized causal Lagrangian is spherically symmetric, also the corresponding demarcation function does not contain any angular dependence. The remaining two paragraphs are concerned with the analysis of the ε-dependence of this demarcation function.

Contour Lines of the iε-Regularized Causal Lagrangian

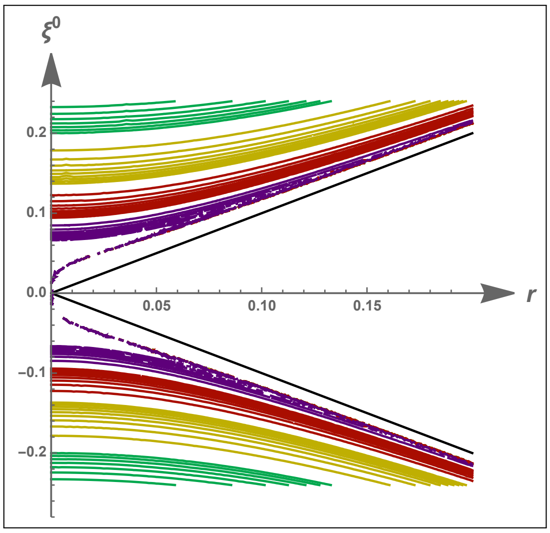
To get a first impression of the ε-dependence of the iε-regularized causal Lagrangian derived in Lemma 2.3.7, we plotted the contour lines $\mathcal{L}^\varepsilon_{\mathrm{h}}(\xi) = \mathrm{const}$ for different values of the constant (see Figure 2.2). Considering only Figure 2.2a for the moment, we recognize a sharp decay of the iε-regularized causal Lagrangian for $\xi^0 \to \pm\infty$ in accordance with the asymptotic expansion of the modified Bessel functions for large arguments.[57, 8.451/6] Analyzing the change of the contour lines from Figure 2.2a to Figure 2.2d, one can see the following three simultaneously occurring effects for decreasing regularization length ε: First, we observe that away from the lightcone (i. e. for $|\xi^0| \gg r$) the bunches of contour lines corresponding to small heights are pushed further outwards. Secondly, near the lightcone (i. e. for $|\xi| \approx r$) the contour lines are “folded” which results in tails approaching the demarcation function and reaching further and further outwards for decreasing regularization length. Finally, the demarcation function (which corresponds to the contour line of height zero) itself converges to the lightcone, but leaves an increasingly thinner tubular-shaped passage between the set of timelike-separated distance vectors ξ with $\xi^0 > 0$ and $\xi^0 < 0$ as long as the regularization length remains positive. These graphics illustrate the fact that the regularization makes the region of spacelike-separated difference vectors larger.[11, Sec. 2.4.1]



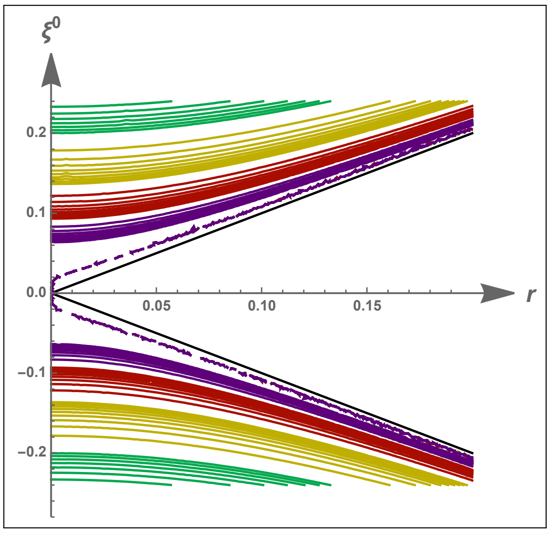
(a) Level sets for $\varepsilon = 10^{-1}$



(b) Level sets for $\varepsilon = 10^{-2}$



(c) Level sets for $\varepsilon = 10^{-3}$



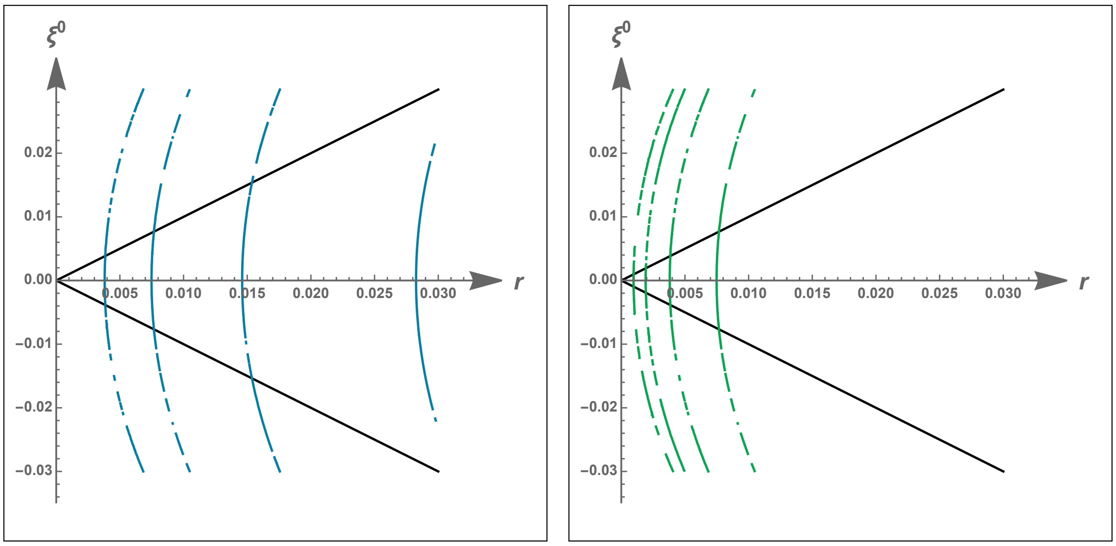
(d) Level sets for $\varepsilon = 10^{-4}$

Figure 2.2: Contour plot of the iε-regularized causal Lagrangian for $\mu = 2\pi$ and different values of the regularization length $\varepsilon \in (0,1)$: The bunches of blue, green, yellow, red and purple contour lines correspond to the contour line sets $\mathcal{C}_{0,0.1}$, $\mathcal{C}_{2,1}$, $\mathcal{C}_{20,10}$, $\mathcal{C}_{200,100}$ and $\mathcal{C}_{2000,1000}$, respectively, which are defined as $\mathcal{C}_{a,d} := \{a + n \cdot d \,|\, a, d \in \mathbb{R}_0^+, n = 0,1,2,\ldots,8\}$. The black line represents the undeformed lightcone $|\xi^0| = r$. Note that the partially discontinuous contour lines are an unavoidable artifact of the plotting process of an implicitly-defined function using `ContourPlot` in Mathematica 12.

Behaviour of the Demarcation Function near the Origin $\xi = 0$

Having developed a basic sense of the behaviour of the iε-regularized causal Lagrangian, we now focus on the region near the origin $\xi = 0$. Plotting the demarcation function for different values of the regularization length ε (see Figure 2.3) and the mass parameter μ (see Figure 2.4), we find that the diameter of the roughly tubular passage connecting timelike-separated distance vectors ξ with $\xi^0 > 0$ and $\xi^0 < 0$ scales like

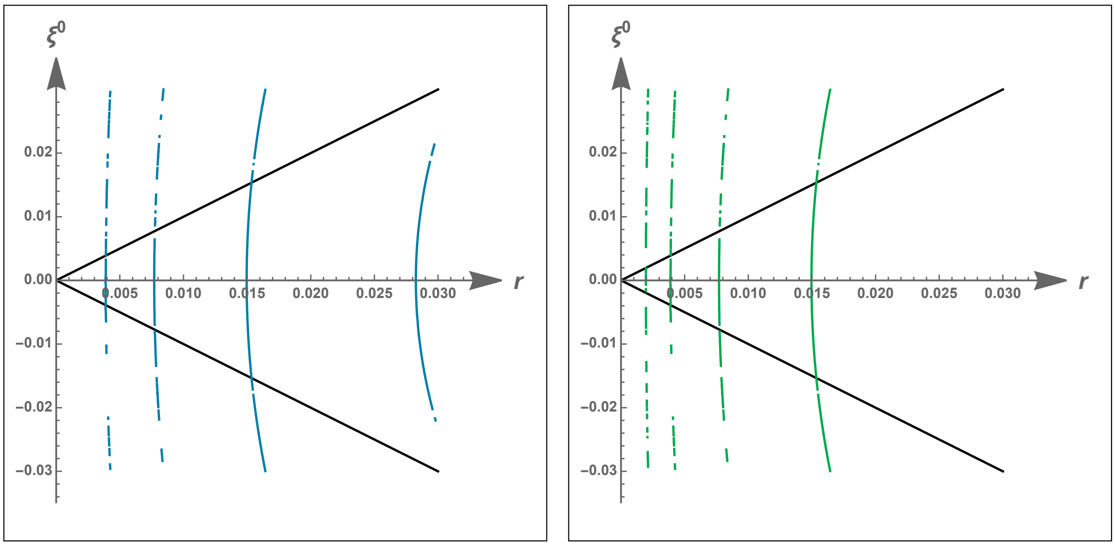
$$\text{diameter} \sim \mu\varepsilon^2 \tag{2.47}$$



(a) Demarcation function for $\mu = 2\pi$ and regularization lengths $\varepsilon \in \mathcal{E}_{0.1,1/\sqrt{2}}$: A decrease of the regularization length by a factor $1/\sqrt{2}$ leads to a decrease of the diameter at the thinnest point by roughly a factor $1/2$.

(b) Demarcation function for $m = 2\pi$ and regularization lengths $\varepsilon \in \mathcal{E}_{0.05,1/\sqrt{2}}$: A decrease of the regularization length by a factor $1/\sqrt{2}$ leads to a decrease of the diameter at the thinnest point by roughly a factor $1/2$.

Figure 2.3: Contour graph of the demarcation function $R^{\varepsilon}_{\text{max}}(\xi^0, r)$ corresponding to the iε-regularized causal Lagrangian for $m = 2\pi$ and different values of the regularization length ε: The bunches of blue and green contour lines correspond to regularization lengths $\varepsilon \in \mathcal{E}_{0.1,1/\sqrt{2}}$ and $\varepsilon \in \mathcal{E}_{0.05,1/\sqrt{2}}$ where the sets are defined as $\mathcal{E}_{\varepsilon_0,q} := \{\varepsilon = \varepsilon_0 \cdot q^n \mid n = 0, 1, 2, 3\}$.



(a) Demarcation function for $\varepsilon = 0.1$ and mass parameter $\mu \in \mathcal{M}_{2\pi,1/2}$: A decrease of the mass parameter by a factor $1/2$ leads to a decrease of the diameter at the thinnest point by roughly a factor $1/2$.

(b) Demarcation function for $\varepsilon = 0.1$ and mass parameter $\mu \in \mathcal{M}_{\pi,1/2}$: A decrease of the mass parameter by a factor $1/2$ leads to a decrease of the diameter at the thinnest point by roughly a factor $1/2$.

Figure 2.4: Contour graph of the demarcation function $R^{\varepsilon}_{\text{max}}(\xi^0, r)$ corresponding to the iε-regularized causal Lagrangian for $\varepsilon = 0.1$ and different values of the mass parameter μ: The bunches of blue and green contour lines correspond to $\mu \in \mathcal{M}_{2\pi,1/2}$ and $\mu \in \mathcal{M}_{\pi,1/2}$ where the sets are defined as $\mathcal{M}_{\mu_0,q} := \{\mu = \mu_0 \cdot q^n \mid n = 0, 1, 2, 3\}$.

at leading order which is in perfect accordance with the scaling of the tubular-shaped region of timelike-separated difference vectors near the origin as derived by Curiel, Finster and Isidro[60, Eq. (A. 13)] A closer numerical examination shows that the scaling behaviour is actually given by

$$\text{diameter} \sim \mu\varepsilon^{2.15} \tag{2.48}$$

Part II

Developments

Variations of the Regularized Causal Action

3

Derivation of the Second Variation of the Regularized Causal Action

Contents

Having introduced the fundamental structures of the theory of causal fermion systems in Chapter 1 and subsequently explained in Chapter 2 how a given physical vacuum system can be modelled within these structures, the present chapter is concerned with the question how modifications of the microstructure of physical spacetime affect the regularized causal action.

As discussed in Subsection 2.2.2.1, the microstructure of physical spacetime $\mathscr{M}$ enters the game via regularization operators $\mathfrak{R}^\varepsilon : \mathcal{H} \to \Gamma(\mathscr{M}, S\mathscr{M})$ from which one can construct the local correlation function $\mathrm{F}^\varepsilon : \mathscr{M} \to \mathcal{F}_n$. This local correlation function, in turn, leads to the regularized kernel of the fermionic projector $\mathrm{P}^\varepsilon \in \Gamma(\mathscr{M} \times \mathscr{M}, S^\varepsilon \boxtimes S^\varepsilon)$ which encodes both the microstructure of physical spacetime as well as the Dirac sea of all negative-frequency solutions of the Dirac equation in the physical spacetime under consideration. Finally, by forming the regularized causal action $\mathcal{S}^\varepsilon$ and varying the regularization, the causal action principle ultimately determines a microstructure which is optimal in the sense that the associated regularized kernel of the fermionic projector minimizes the regularized causal action. This being said, it becomes clear that analyzing how deformations of the microstructure of physical spacetime affect the regularized causal action, requires to derive expressions for the variation of the regularized causal action in terms of the variation of the regularized kernel of the fermionic projector. Based on this, one can subsequently study how initial perturbations of the microstructure lead to a dynamics aimed at realizing a new optimal microstructure of physical spacetime. This will be discussed in more detail in Chapter 5 and there, in particular, in Section 5.3.

3.1 Basics of the Calculus of Variations

We start by introducing the necessary definitions required to formalize what exactly we mean when talking about variations of the regularized causal action. According to Definition 2.2.17 (Causal Action Evaluation Operator), the regularized causal action can be interpreted as the outcome of the mapping

$$\Sigma : \Gamma(\mathscr{M} \times \mathscr{M}, S^\varepsilon \boxtimes S^\varepsilon) \to \mathbb{R}_0^+ \quad \text{with} \quad \mathrm{P}^\varepsilon \mapsto \Sigma[\mathrm{P}^\varepsilon] := \mathcal{S}^\varepsilon \tag{3.1}$$

In the cases relevant for us, namely in the setting where the underlying Lorentzian manifold is given by Minkowski space $(\mathscr{M}, \eta)$ and the regularized kernel of the fermionic projector is homogeneous, we are actually working with mappings $\mathrm{P}^\varepsilon \in C^\infty(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4, \mathbb{C}^4))$.

In order to define what is meant by a variation of the causal action, it is instructive to briefly review the definitions of variations commonly used in the literature. The simplest setting considered in the classical calculus of variations is clearly the one where (real-valued) functions defined on an open subset of $\mathbb{R}^n$ are analyzed by calculating first variations which in this case are realized as ordinary directional derivatives. In more general situations one deals with functionals defined on Banach spaces or even with functional defined on normed vector spaces. In both cases, first and higher-order variations of the functionals are realized by generalizing the notion of ordinary directional derivatives to Gâteaux derivatives.[61, Ch. 2, Appendix]

Definition 3.1.1 (Gâteaux Differentiability and Gâteaux Derivative)

Let $(X, \|\cdot\|_X)$ and $(Y, \|\cdot\|_Y)$ be normed vector spaces and let $U \in \mathcal{T}_{\|\cdot\|_X}$ be an open set of X where $\mathcal{T}_{\|\cdot\|_X}$ denotes the norm-induced topology on X. A function $f : U \to Y$ is called *Gâteaux differentiable at* $x_0 \in U$ if the limit

$$\left.\frac{\mathrm{d}f(x_0 + \tau v)}{\mathrm{d}\tau}\right|_{\tau=0} := \lim_{\tau \to 0} \frac{f(x_0 + \tau v) - f(x_0)}{\tau} \tag{3.2}$$

referred to as the *directional derivative of* f *at* x_0 *in the direction* v, exists for all directions $v \in X$ and if there is a continuous linear mapping $df(x_0) \in \mathrm{L}(X, Y)$, referred to as the *Gâteaux derivative of* f *at* $x_0 \in U$, such that

$$\left.\frac{\mathrm{d}f(x_0 + \tau v)}{\mathrm{d}\tau}\right|_{\tau=0} = \big(df(x_0)\big)(v) \tag{3.3}$$

Remark 3.1.2 (Gâteaux Derivative)

We remark that there is no consensus in the literature, neither regarding the definition of Gâteaux differentiability nor regarding terminology: While some authors[61],[62, App. A] introduce the Gâteaux differential/derivative as presented in Definition 3.1.1 and thus follow the later works by Gâteaux[63, Sec. 3], other authors[64, Sec. 2.1C] drop the requirement of $df(x_0)$ being continuous and linear (while keeping homogeneity of degree one) which is more in accordance with Gâteaux's original definition.[65] To distinguish between both situations, some authors refer to $df(x_0)$ as the Gâteaux *differential* and reserve the term Gâteaux *derivative* for the case where $df(x_0)$ is continuous and linear.

By employing the machinery of differential calculus on topological vector spaces,[1] one can even consider functionals defined on topological vector spaces which, in particular, covers the case of functionals defined on Fréchet spaces. In this case which will be relevant for our purposes (see below in Section 3.4), variations can be defined in terms of a generalized version of Gâteaux derivatives which is consistently referred to as directional derivatives in the literature.[66, p. 6],[68, Sec. I.3]

[1] For details we refer to the textbook by Yamamuro.[66] For a treatment which uses so-called *convenient vector spaces*, we refer to the textbook by Kriegl and Michor.[67, Sec. 13]

Definition 3.1.3 (Directional Derivative on Topological Vector Spaces)

Let $(X, \mathcal{T}_X)$ and $(Y, \mathcal{T}_Y)$ be topological vector spaces over the real numbers $\mathbb{R}$ and let $U \in \mathcal{T}_X$ be an open set of X. A function $f : U \to Y$ is called *differentiable at $x_0 \in U$ in the direction $v \in X$* if the limit

$$\big(df(x_0)\big)(v) := \frac{\mathrm{d}f(x_0 + \tau v)}{\mathrm{d}\tau}\bigg|_{\tau=0} := \lim_{\tau\to 0} \frac{f(x_0+\tau v) - f(x_0)}{\tau} \tag{3.4}$$

referred to as the *directional derivative of f at x_0 in the direction $v \in X$*, exists.

With this definition of differentiability at hand, we can now formalize what in the classical calculus of variations is usually referred to as the first variation of a functional on some function space.[2]

Definition 3.1.4 (First and Second Variation of a Functional)

Let $J : X \to Y$ be a mapping between topological vector spaces X, Y and let $\gamma : (-\tau_0, \tau_0) \to X$ for $\tau_0 > 0$ be a smooth curve in X. Then the *first variation δJ of J at $x_0 \in X$ evaluated at* $v := \gamma'(0)$ is defined as

$$\big(\delta J(x_0)\big)(v) := \frac{\mathrm{d}\Phi(\tau)}{\mathrm{d}\tau}\bigg|_{\tau=0} \qquad \text{where} \qquad \Phi := J \circ \gamma \tag{3.5a}$$

Likewise, the *second variation $\delta^2 J$ of J at $x_0 \in X$ evaluated at $v = \gamma'(0)$ and $w := \gamma''(0)$* is defined as

$$\big(\delta^2 J(x_0)\big)(v, w) := \frac{1}{2}\frac{\mathrm{d}^2\Phi(\tau)}{\mathrm{d}\tau^2}\bigg|_{\tau=0} \tag{3.5b}$$

Before we apply this definition to concrete examples, we shall at least briefly discuss the relationship of these variations in the case $Y = \mathbb{R}$ with the definition of the first and second variations as commonly used in the classical calculus of variations. Carrying out the derivative in the definition of the first variation and using the chain rule we obtain

$$\big(\delta J(x_0)\big)(v) \overset{(3.5a)}{=} \frac{\mathrm{d}\Phi(\tau)}{\mathrm{d}\tau}\bigg|_{\tau=0} = (d_{\gamma(0)}J)\big(\gamma'(0)\big) = (d_{x_0}J)(v) \tag{3.6}$$

where $(d_{x_0}J)(v)$ denotes the directional derivative of J at x_0 in the direction v. This result coincides with the definition of the first variation in the standard textbooks on the classical calculus of variations. If we now interpret $(d_{\gamma(\tau)}J)\big(\gamma'(\tau)\big)$ as a real-valued function $\Psi : (-\tau_0, \tau_0) \to \mathbb{R}$ and use the chain rule once more, the second variation of J can be expressed as

$$\big(\delta^2 J(x_0)\big)(v, w) \overset{(3.5b)}{=} \frac{1}{2}\frac{\mathrm{d}\Psi(\tau)}{\mathrm{d}\tau}\bigg|_{\tau=0} = \frac{1}{2}\big(d^2_{\gamma(0)}J\big)\big(\gamma'(0), \gamma'(0)\big) + \frac{1}{2}(d_{\gamma(0)}J)(\gamma''(0)) \tag{3.7}$$

The first term in this expression is the second directional derivative of J at $x_0 = \gamma(0)$ in the direction $v = \gamma'(0)$ what in the classical calculus of variations is referred to as *the* second variation.[16, Sec. 24] The additional term, namely the first directional derivative at $x_0 = \gamma(0)$ in the direction $\gamma''(0)$ is absent in classical treatments. For a thorough study of second variations which takes into account all contributions at second order, however, this term must be included.

[2]For the classical calculus of variations, we refer to the standard literature, namely the textbooks by Courant and Hilbert[69, Ch. 4] as well as the one by Gel'fand and Fomin[16, Sec. 3.2]. To complement both, we also recommend the textbook by Giaquinta and Hildebrandt where the connection between derivatives and variations is discussed.[70, p. 9-11]

3.2 Foundational Assumptions on P^ε

In Subsection 2.3.2 we introduced the iε-regularized kernel of the fermionic projector which is a special case of Definition 2.2.13. In order to clarify the assumptions on the class of regularized kernels of the fermionic projector which will be considered in this and the following chapters, we list and briefly comment on them below.

Homogeneity of the Regularized Kernel of the Fermionic Projector
In the case where physical spacetime is given by Minkowski space $(\mathscr{M}, \eta)$, we assume that the regularized kernel of the fermionic projector is homogeneous in the sense that it does not depend on the pair $x, y \in \mathscr{M}$ of physical spacetime points themselves, but rather on their difference vector $\xi := y - x$ and in this way preserves translation invariance of Minkowski spacetime.

Assumption 3.2.1 (Homogeneity of P^ε)

Whenever physical spacetime is given by Minkowski space $(\mathscr{M}, \eta)$, we assume that the regularized kernel of the fermionic projector $\mathrm{P}^\varepsilon \in \Gamma^\infty(\mathscr{M} \times \mathscr{M}, S^\varepsilon \boxtimes S^\varepsilon)$ is the section which, upon evaluation at $(x, y) \in \mathscr{M} \times \mathscr{M}$ is homogeneous in the sense that it only depends on the difference vector $\xi := y - x$ rather than on the spacetime points $x, y \in \mathscr{M}$ themselves[a]

$$\mathrm{P}^\varepsilon(x, y) = \mathrm{P}^\varepsilon(y - x) \tag{3.8}$$

In this case, as already discussed in Subsection 2.3.2, the regularized kernel of the fermionic projector is regarded as a function $\mathrm{P}^\varepsilon \in C^\infty(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4, \mathbb{C}^4))$.

[a] As we exclusively consider homogeneous regularized kernels of the fermionic projector in all subsequent chapters, we commit the mild sin of using the same symbol.

More generally speaking, homogeneity actually only requires that physical spacetime carries a vector space structure in order for the difference vector to be defined at all. The second physically relevant case besides Minkowski space which is discussed in the literature is the *discrete case* where one considers a periodic lattice in Minkowski spacetime.[7, Sec. 4],[12]

Vector-Scalar Structure of the Regularized Kernel of the Fermionic Projector
According to the discussion of the foundational conceptions underlying the modelling of physical systems within the framework of causal fermion systems and based on Assumption 2.2.1, we constructed the regularized kernel of the fermionic projector from the local correlation function which encodes both the regularization as well as the Dirac sea interpretation of the entirety of negative-energy solutions of the Dirac equation. Later on, by restricting to Minkowski spacetime and choosing the iε-regularization, we arrived at the iε-regularized kernel of the fermionic projector which inherits its vector-scalar structure from the Dirac equation. Now, since there is no experimental evidence which strongly suggests or even requires a modification of the Dirac equation (except, maybe, at high energies which are not accessible to current accelerators), we assume that *any* regularization preserves this vector-scalar structure.[3]

Assumption 3.2.2 (Vector-Scalar Structure of P^ε)

Throughout all following chapters, we assume that the homogeneous regularized kernel of the fermionic projector $\mathrm{P}^\varepsilon \in C^\infty(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4, \mathbb{C}^4))$, upon evaluation at $\xi \in \mathbb{R}^4$, has the special form

$$\xi \mapsto \mathrm{P}^\varepsilon(\xi) = \sum_{i=0}^{3} v_i^\varepsilon(\xi)\gamma^i + s^\varepsilon(\xi)\mathrm{id}_{\mathbb{C}^4} \tag{3.9}$$

[3] For a more detailed discussion concerning the vector-scalar structure of the regularized kernel of the fermionic projector, we refer to the last paragraph in section 4.1 of Finster's first book.[6, Sec. 4.1]

referred to as *vector-scalar structure* of the regularized kernel of the fermionic projector.[a] The γ^i (for $i \in \{0,1,2,3\}$) denote the Dirac matrices and the coefficient functions $v_i^\varepsilon \in C^\infty(\mathbb{R}^4, \mathbb{C})$ and $s^\varepsilon \in C^\infty(\mathbb{R}^4, \mathbb{C})$ are the so-called *vector components* and the *scalar component* of the regularized kernel of the fermionic projector, respectively.

[a]This terminology was introduced by Finster.[6, p. 94],[11, p. 32]

We note that the function space $C^\infty(\mathbb{R}^4, \mathbb{C})$ must be replaced by a suitable Fréchet space when variations of the regularized causal action are considered. In this case we have to interpret $\mathcal{S}_\mathrm{h}^\varepsilon$ as the functional Σ_h which takes P^ε as input. We will come back to this issue in Section 3.4.

Shape of the Region of Non-Spacelike Separated Difference Vectors

Finally, the third foundational assumption does not concern the structure of the regularized kernel of the fermionic projector, but rather the choice of the regularization itself.

Assumption 3.2.3 (Shape of the Region $\mathcal{R}^\varepsilon$)

Whenever physical spacetime is given by Minkowski space $(\mathscr{M}, \eta)$ and the regularized kernel of the fermionic projector is homogeneous, we assume that the regularization is chosen such that the region of non-spacelike separated difference vectors

$$\mathcal{R}^\varepsilon := \left\{ \xi \in \mathbb{R}^4 \,\middle|\, \mathcal{L}_\mathrm{h}^\varepsilon(\xi) > 0 \right\} \tag{3.10}$$

is simply connected and that for every $a \in \mathbb{R}$ the subset $\mathcal{R}_a^\varepsilon := \{\xi^4 \in \mathcal{R}^\varepsilon \,|\, \xi^0 = a\}$ is star-shaped.

The assumption on the shape of the region $\mathcal{R}^\varepsilon$ ensures that the set of timelike-separated difference vectors does not split into two or more connected components, prevents an enclave of spacelike-separated difference vectors within $\mathcal{R}^\varepsilon$ and guarantees that the demarcation function is sufficiently well-behaved.

Relation to Regularizations in the Literature As already mentioned in the paragraph on the choice of the regularization operators in the case of the Minkowski vacuum, the study of regularizations different from the iε-regularization comes at the cost of considerable technical effort. For this reason, there is essentially only one paper[71] that systematically analyzes the effect of the choice of the regularization on the regularized causal Lagrangian and the regularized causal action.[4] More concretely, the paper considers a class of homogeneous, spherically-symmetric regularized kernels of the fermionic projector which have vector-scalar structure and are composed of so-called *surface states*. The detailed analysis in the different regions of physical spacetime referred to as the *outer strip*, *intermediate layers* and *inner layers* unveils a highly complicated shape of the set of non-spacelike separated difference vectors $\xi \in \mathbb{R}^4$.

Compared with this, our assumption on the shape of the region $\mathcal{R}^\varepsilon$ aims in a different direction: Instead of spherically-symmetric homogeneous regularized kernels of the fermionic projector composed of surface states, we will ultimately consider anisotropically iε-regularized kernels of the fermionic projector.

Notation 3.2.4 (Homogeneity)

Unless otherwise stated, the regularized kernel of the fermionic projector, the regularized closed chain, the regularized causal Lagrangian and the regularized causal action are from now on assumed to be homogeneous.

[4]Besides the paper by Finster[71], there is another paper by Curiel, Finster and Isidro[60, App. A] in which the scaling of the regularized causal Lagrangian is studied.

3.3 The Regularized Closed Chain

As already explained in Subsection 1.4.1, the closed chain A_{xy} plays the central role in the calculation of the eigenvalues λ_i^{xy} of operator products xy for $x, y \in \mathcal{F}_n$ which in turn serve as the building blocks of the causal Lagrangian. In this section, starting from a homogeneous regularized kernel P^ε of the fermionic projector with vector-scalar structure, we derive explicit expressions for the corresponding regularized closed chain $A^\varepsilon(x,y)$, its eigenvalues $\lambda_i^\varepsilon(x,y)$ as well as the corresponding spectral projectors. Before, however, we take the opportunity to introduce abbreviations for frequently occurring combinations of the vector and scalar component of the regularized kernel of the fermionic projector.

Notation 3.3.1 (Combinations of the Vector and Scalar Components of P^ε)

Given the symmetry of the kernel of the fermionic projector with respect to the spin space inner product, the vector and scalar components of its adjoint, namely the complex-conjugates $\overline{v_i^\varepsilon}(\xi), \overline{s^\varepsilon}(\xi)$, can be expressed in terms of vector and scalar components of a homogeneous regularized kernel of the fermionic projector as

$$\overline{v_i^\varepsilon}(\xi) = v_i^\varepsilon(-\xi) \qquad (3.11a) \qquad\qquad \overline{s^\varepsilon}(\xi) = s^\varepsilon(-\xi) \qquad (3.11b)$$

In addition to this, we introduce combinations of the vector and scalar components as functions $(v^\varepsilon)^2, (\overline{v^\varepsilon})^2, (s^\varepsilon)^2, (\overline{v^\varepsilon})^2 \in C^\infty(\mathbb{R}^4, \mathbb{C})$ and $|v^\varepsilon|^2, |s^\varepsilon|^2 \in C^\infty(\mathbb{R}^4, \mathbb{R})$ which are defined as follows

$$(v^\varepsilon)^2 := \eta^{ij} v_i^\varepsilon v_j^\varepsilon \quad (3.12a) \qquad (\overline{v^\varepsilon})^2 := \eta^{ij} \overline{v_i^\varepsilon}\,\overline{v_j^\varepsilon} \quad (3.12b) \qquad |v^\varepsilon|^2 := \eta^{ij} v_i^\varepsilon \overline{v_j^\varepsilon} \quad (3.12c)$$

$$(s^\varepsilon)^2 := s^\varepsilon s^\varepsilon \quad (3.12d) \qquad (\overline{s^\varepsilon})^2 := \overline{s^\varepsilon}\,\overline{s^\varepsilon} \quad (3.12e) \qquad |s^\varepsilon|^2 := s^\varepsilon \overline{s^\varepsilon} \quad (3.12f)$$

After these preparations, we now derive an expression for the regularized closed chain.

Lemma 3.3.2 (Decomposition of the Regularized Closed Chain)

Let $\mathrm{P}^\varepsilon \in C^\infty(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4, \mathbb{C}^4))$ be a homogeneous regularized kernel of the fermionic projector which has vector-scalar structure. Then the regularized closed chain can be decomposed as

$$A^\varepsilon(x,y) = A_{ij}^\varepsilon(\xi)[\gamma^i, \gamma^j] + A_i^\varepsilon(\xi)\gamma^i + A_\mathrm{s}^\varepsilon(\xi)\mathrm{id}_{\mathbb{C}^4} \qquad (3.13)$$

where the functions $A_{ij}^\varepsilon \in C^\infty(\mathbb{R}^4, \mathbb{C})$ and $A_i^\varepsilon, A_\mathrm{s}^\varepsilon \in C^\infty(\mathbb{R}^4, \mathbb{R})$ referred to as the *bilinear*, *vector* and *scalar component* of the regularized closed chain, respectively, are given by

$$A_{ij}^\varepsilon = \frac{1}{2} v_i^\varepsilon \overline{v_j^\varepsilon} \quad (3.13a) \qquad A_i^\varepsilon = 2\,\mathrm{Re}\,(v_i^\varepsilon \overline{s^\varepsilon}) \quad (3.13b) \qquad A_\mathrm{s}^\varepsilon = |v^\varepsilon|^2 + |s^\varepsilon|^2 \quad (3.13c)$$

Proof. Inserting the vector-scalar structure of the regularized kernel of the fermionic projector into the definition of the regularized closed chain from Definition 2.2.12 yields

$$\begin{aligned} A^\varepsilon(x,y) &\overset{(2.19)}{=} \left(v_i^\varepsilon(\xi)\gamma^i + s^\varepsilon(\xi)\mathrm{id}_{\mathbb{C}^4}\right)\left(v_j^\varepsilon(-\xi)\gamma^j + s^\varepsilon(-\xi)\mathrm{id}_{\mathbb{C}^4}\right) \\ &= v_i^\varepsilon(\xi)v_j^\varepsilon(-\xi)\gamma^i\gamma^j + \left(v_i^\varepsilon(\xi)s^\varepsilon(-\xi) + s^\varepsilon(\xi)v_i^\varepsilon(-\xi)\right)\gamma^i + s^\varepsilon(\xi)s^\varepsilon(-\xi)\mathrm{id}_{\mathbb{C}^4} \end{aligned}$$

Decomposing the product of Dirac matrices by using the defining relation of the Clifford algebra of the Dirac matrices

$$\gamma^i\gamma^j = \frac{1}{2}[\gamma^i, \gamma^j] + \frac{1}{2}\{\gamma^i, \gamma^j\} = \frac{1}{2}[\gamma^i, \gamma^j] + \eta^{ij}\mathrm{id}_{\mathbb{C}^4}$$

and furthermore making use of the relations $v_i^\varepsilon(-\xi) = \overline{v_i^\varepsilon}(\xi)$ and $s^\varepsilon(-\xi) = \overline{s^\varepsilon}(\xi)$ which follow from the symmetry properties of the (regularized) kernel of the fermionic projector, leads to

$$\begin{aligned} \dots &= \frac{1}{2} v_i^\varepsilon(\xi)\overline{v_j^\varepsilon}(\xi)[\gamma^i,\gamma^j] + \big(v_i^\varepsilon(\xi)\overline{s^\varepsilon}(\xi) + s^\varepsilon(\xi)\overline{v_i^\varepsilon}(\xi)\big)\gamma^i + \big(\eta^{ij} v_i^\varepsilon(\xi)\overline{v_j^\varepsilon}(\xi) + s^\varepsilon(\xi)\overline{s^\varepsilon}(\xi)\big)\mathrm{id}_{\mathbb{C}^4} \\ &= \frac{1}{2} v_i^\varepsilon(\xi)\overline{v_j^\varepsilon}(\xi)[\gamma^i,\gamma^j] + 2\,\mathrm{Re}\,\big(v_i^\varepsilon(\xi)\overline{s^\varepsilon}(\xi)\big)\gamma^i + \big(|v^\varepsilon|^2(\xi) + |s^\varepsilon|^2(\xi)\big)\mathrm{id}_{\mathbb{C}^4} \end{aligned}$$

Identifying the first and second term as the bilinear and vector contribution, respectively, and the last term as the scalar part concludes this short proof. ☐

At this point we introduce one more frequently occurring combination combination of the vector and scalar components of the regularized kernel of the fermionic projector.

Definition 3.3.3 (Regularized Discriminant)

The *regularized discriminant*[a] $\mathcal{D}^\varepsilon \in C^\infty(\mathbb{R}^4,\mathbb{R})$ is defined as

$$\mathcal{D}^\varepsilon(\xi) := \big(B^\varepsilon(\xi)\big)^2 - \big|C^\varepsilon(\xi)\big|^2 \tag{3.14}$$

where the functions $B^\varepsilon \in C^\infty(\mathbb{R}^4,\mathbb{R})$ and $C^\varepsilon \in C^\infty(\mathbb{R}^4,\mathbb{C})$ are given by

$$B^\varepsilon(\xi) := |v^\varepsilon|^2(\xi) + |s^\varepsilon|^2(\xi) \tag{3.15a}$$

$$C^\varepsilon(\xi) := (\overline{v^\varepsilon})^2(\xi) - (\overline{s^\varepsilon})^2(\xi) \tag{3.15b}$$

[a] As will become clear in Lemma 3.3.4, the terminology is motivated by the fact that $\mathcal{D}^\varepsilon$ appears as the radicand in the expression for the eigenvalues of the regularized closed chain.

3.3.1 Eigenvalues of the Regularized Closed Chain

Having derived the form of the regularized closed chain in the case where the regularized kernel of the fermionic projector has vector-scalar structure, we now turn to the computation of the eigenvalues of $A^\varepsilon(x,y)$.

Lemma 3.3.4 (Eigenvalues of the Regularized Closed Chain)

Let $A^\varepsilon(x,y)$ be the regularized closed chain as derived in Lemma 3.3.2. In this case, its eigenvalues are given by

$$\lambda_\pm^\varepsilon(x,y) = B^\varepsilon(\xi) \pm \mathcal{D}^\varepsilon(\xi)^{1/2} \tag{3.16}$$

where B^ε and $\mathcal{D}^\varepsilon$ are the functions introduced in Definition 3.3.3.

Proof. In order to find the roots of the regularized closed chain $A^\varepsilon(x,y)$ as given in Lemma 3.3.2, we derive a quadratic matrix equation for $A^\varepsilon(x,y)$ by exploiting the properties of the Dirac matrices. Taking the square of the trace-free part of $A^\varepsilon(x,y)$ and suppressing arguments results in

$$\left(A^\varepsilon(x,y) - \frac{1}{4}\,\mathrm{Tr}\left[A^\varepsilon(x,y)\right]\mathrm{id}_{\mathbb{C}^4}\right)^2 \overset{(3.13)}{=} A_{ij}^\varepsilon A_{kl}^\varepsilon[\gamma^i,\gamma^j][\gamma^k,\gamma^l] + A_{ij}^\varepsilon A_k^\varepsilon\left\{[\gamma^i,\gamma^j],\gamma^k\right\} + A_i^\varepsilon A_j^\varepsilon\gamma^i\gamma^j$$

Here we exploited the fact that the trace of a single Dirac matrix as well as the trace of the commutator of two Dirac matrices both vanish identically. The products of Dirac matrices in the first and second term can be rewritten as

$$[\gamma^i,\gamma^j][\gamma^k,\gamma^l] = 2(\eta^{jk}\gamma^i\gamma^l + \eta^{il}\gamma^j\gamma^k) - \{(\gamma^i\gamma^k),(\gamma^j\gamma^l)\} - \gamma^j(\gamma^i\gamma^k)\gamma^l - \gamma^i(\gamma^j\gamma^l)\gamma^k$$
$$\{[\gamma^i,\gamma^j],\gamma^k\} = 2(\gamma^i\gamma^k\gamma^j - \gamma^j\gamma^k\gamma^i)$$

where we repeatedly used the defining relation $\{\gamma^i,\gamma^j\} = 2\eta^{ij}\mathrm{id}_{\mathbb{C}^4}$ of the Clifford algebra of the Dirac matrices. Inserting these relations into the above equation and using the identity $a_i a_j \gamma^i\gamma^j = \eta^{ij}a_i a_j = a^2$ yields

$$\begin{aligned}
&\left(A^\varepsilon(x,y) - \frac{1}{4}\operatorname{Tr}\left[A^\varepsilon(x,y)\right]\mathrm{id}_{\mathbb{C}^4}\right)^2 = \\
&\overset{(3.13)}{\underset{(3.17)}{=}} \frac{1}{2}|v^\varepsilon|^2\left(v_i^\varepsilon\overline{v_l^\varepsilon}\gamma^i\gamma^l + \overline{v_j^\varepsilon}v_k^\varepsilon\gamma^j\gamma^k\right) - (v^\varepsilon)^2(\overline{v^\varepsilon})^2\mathrm{id}_{\mathbb{C}^4} \\
&\quad + \underbrace{v_i^\varepsilon\gamma^i(\overline{v^\varepsilon})^2 s^\varepsilon}_{(1)} + \underbrace{\overline{v_j^\varepsilon}\gamma^j(v^\varepsilon)^2\overline{s^\varepsilon}}_{(2)} - \underbrace{v_i^\varepsilon\gamma^i(\overline{v^\varepsilon})^2 s^\varepsilon}_{\text{cancels (1)}} - \underbrace{\overline{v_j^\varepsilon}\gamma^j(v^\varepsilon)^2\overline{s^\varepsilon}}_{\text{cancels (2)}} \\
&\quad + \left((\overline{v^\varepsilon})^2(s^\varepsilon)^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (v^\varepsilon)^2(\overline{s^\varepsilon})^2\right)\mathrm{id}_{\mathbb{C}^4} \\
&= \left(\left(|v^\varepsilon|^2\right)^2 - (v^\varepsilon)^2(\overline{v^\varepsilon})^2 + 2\operatorname{Re}\left[(\overline{v^\varepsilon})^2(s^\varepsilon)^2\right] + 2|v^\varepsilon|^2|s^\varepsilon|^2\right)\mathrm{id}_{\mathbb{C}^4}
\end{aligned}$$

where we recognize the regularized discriminant $\mathcal{D}^\varepsilon$ as introduced in (3.14). In this way we find that the regularized closed chain has to satisfy the following quadratic matrix equation

$$\left(A^\varepsilon(x,y) - \frac{1}{4}\operatorname{Tr}\left[A^\varepsilon(x,y)\right]\mathrm{id}_{\mathbb{C}^4}\right)^2 = \mathcal{D}^\varepsilon(\xi)\mathrm{id}_{\mathbb{C}^4}$$

Bringing both terms to the left-hand side, inserting the trace of the regularized closed chain which evaluates to $\frac{1}{4}\operatorname{Tr}\left[A^\varepsilon(x,y)\right] = A_\mathrm{s}^\varepsilon(\xi) = |v^\varepsilon|^2(\xi) + |s^\varepsilon|^2(\xi) = B^\varepsilon(\xi)$ as can be easily seen from (3.13), factorizing and taking the determinant yields

$$0 = \det\left\{\left[A^\varepsilon(x,y) - \left(B^\varepsilon(\xi) + \mathcal{D}^\varepsilon(\xi)^{1/2}\right)\mathrm{id}_{\mathbb{C}^4}\right]\left[A^\varepsilon(x,y) - \left(B^\varepsilon(\xi) - \mathcal{D}^\varepsilon(\xi)^{1/2}\right)\mathrm{id}_{\mathbb{C}^4}\right]\right\}$$

This equation is a condition on the regularized closed chain which is satisfied if the regularized closed chain solves the equations

$$\begin{aligned}
&0 = \det\left[A^\varepsilon(x,y) - \left(B^\varepsilon(\xi) + \mathcal{D}^\varepsilon(\xi)^{1/2}\right)\mathrm{id}_{\mathbb{C}^4}\right] \\
\vee\qquad &0 = \det\left[A^\varepsilon(x,y) - \left(B^\varepsilon(\xi) - \mathcal{D}^\varepsilon(\xi)^{1/2}\right)\mathrm{id}_{\mathbb{C}^4}\right]
\end{aligned}$$

But these equations are just the conditions for $B^\varepsilon(\xi) \pm \mathcal{D}^\varepsilon(\xi)^{1/2}$ to be the roots of the characteristic polynomial of $A^\varepsilon(x,y)$, that is the eigenvalues $\lambda_\pm^\varepsilon(x,y)$.

This concludes the proof. □

3.3.2 Regularized Spectral Projectors

In order to be able to derive the first and second variations of the regularized eigenvalues in Subsection 3.3.3, we need the spectral projectors.

Lemma 3.3.5 (Spectral Projectors)

Let $A^\varepsilon(x,y)$ be the regularized closed chain as derived in Lemma 3.3.2 and let $\lambda_\pm^\varepsilon(x,y)$ be the corresponding eigenvalues from Lemma 3.3.4. Then the regularized spectral projectors $F_\pm^\varepsilon(x,y)$

on the eigenspaces corresponding to the eigenvalue $\lambda_i^\varepsilon(x,y)$, expressed in terms of the components $v_i^\varepsilon, s^\varepsilon$ of the regularized kernel of the fermionic projector as given in Assumption 3.2.2, take the form

$$F_\pm^\varepsilon(x,y) = F_{\pm,ij}^\varepsilon(\xi)[\gamma^i,\gamma^j] + F_{\pm,i}^\varepsilon(\xi)\gamma^i + F_{\pm,\mathrm{s}}^\varepsilon(\xi)\mathrm{id}_{\mathbb{C}^4} \tag{3.18}$$

where the *scalar*, *vector* and *bilinear* components are given by

$$F_{\pm,ij}^\varepsilon = \pm\frac{1}{4}\frac{v_i^\varepsilon \overline{v_j^\varepsilon}}{\sqrt{\mathcal{D}^\varepsilon}} \quad \text{(3.18a)} \qquad F_{\pm,i}^\varepsilon = \pm\frac{\mathrm{Re}(v_i^\varepsilon \overline{s^\varepsilon})}{\sqrt{\mathcal{D}^\varepsilon}} \quad \text{(3.18b)} \qquad F_{\pm,\mathrm{s}}^\varepsilon = \frac{1}{2} \quad \text{(3.18c)}$$

Proof. The spectral projectors are defined as the Frobenius covariants[72, Sec. 1.10] of the regularized closed chain $A^\varepsilon(x,y)$ corresponding to the eigenvalues $\lambda_\pm^\varepsilon(x,y)$

$$F_\pm^\varepsilon(x,y) = \frac{A^\varepsilon(x,y) - \lambda_\mp^\varepsilon(x,y)\mathrm{id}_{\mathbb{C}^4}}{\lambda_\pm^\varepsilon(x,y) - \lambda_\mp^\varepsilon(x,y)}$$

Suppressing arguments and rewriting the expression by inserting $0 = \lambda_\pm^\varepsilon - \lambda_\pm^\varepsilon$ in the numerator yields

$$F_\pm^\varepsilon(x,y) = \frac{A^\varepsilon}{\lambda_\pm^\varepsilon - \lambda_\mp^\varepsilon} - \frac{1}{2}\left(\frac{\lambda_\mp^\varepsilon + \lambda_\pm^\varepsilon}{\lambda_\pm^\varepsilon - \lambda_\mp^\varepsilon} + \frac{\lambda_\mp^\varepsilon - \lambda_\pm^\varepsilon}{\lambda_\pm^\varepsilon - \lambda_\mp^\varepsilon}\right)\mathrm{id}_{\mathbb{C}^4} = \frac{1}{2}\left(\mathrm{id}_{\mathbb{C}^4} + \frac{2A^\varepsilon - \left(\lambda_\mp^\varepsilon + \lambda_\pm^\varepsilon\right)\mathrm{id}_{\mathbb{C}^4}}{\lambda_\pm^\varepsilon - \lambda_\mp^\varepsilon}\right)$$

Inserting expression for the eigenvalues as derived in Lemma 3.3.4 and restoring the arguments results in

$$F_\pm^\varepsilon(x,y) \overset{(3.16)}{=} \frac{1}{2}\left(\mathrm{id}_{\mathbb{C}^4} \pm \frac{2A^\varepsilon(x,y) - 2\left(|v^\varepsilon|^2 + |s^\varepsilon|^2\right)\mathrm{id}_{\mathbb{C}^4}}{2\sqrt{\mathcal{D}^\varepsilon}}\right) \tag{3.19}$$

Finally, be observing that the term $|v^\varepsilon|^2 + |s^\varepsilon|^2$ appearing in the numerator cancels the scalar component in the regularized closed chain, we end up with

$$F_\pm^\varepsilon(x,y) = \frac{1}{2}\left(\mathrm{id}_{\mathbb{C}^4} \pm \frac{A_{ij}^\varepsilon(\xi)[\gamma^i,\gamma^j] + A_i^\varepsilon(\xi)\gamma^i}{\sqrt{\mathcal{D}^\varepsilon(\xi)}}\right) \tag{3.20}$$

Inserting the components of the regularized closed chain as calculated in Lemma 3.3.2 concludes the proof. ☐

Having completed the calculation of the eigenvalues of the regularized closed chain in terms of the vector and scalar components of the homogeneous regularized kernel of the fermionic projector, we next derive the variation of the eigenvalues which are caused by variations of the regularized kernel of the fermionic projector.

3.3.3 Variation of the Eigenvalues of the Regularized Closed Chain

An important intermediate step in deriving expressions for $\delta\mathcal{S}^\varepsilon$ and $\delta^2\mathcal{S}^\varepsilon$ is to calculate the variations of the eigenvalues of the regularized closed chain which ultimately enter these expressions via the variations $\delta\mathcal{L}^\varepsilon$ and $\delta^2\mathcal{L}^\varepsilon$. As will be explained in more detail in the proof of Theorem 3.4.3, the variations of the regularized causal action in the sense of Definition 3.1.4 must actually be regarded as variations $\delta\Sigma_\mathrm{h}$ and $\delta^2\Sigma_\mathrm{h}$ of the causal action evaluation operator introduced in Definition 2.2.17 which maps P^ε to $\mathcal{S}^\varepsilon$. Similarly, also variations of other objects such as the regularized causal Lagrangian, the regularized closed chain and its eigenvalues, which are all built from P^ε, must be regarded as variations of the corresponding evaluation operators. However, in order not to unnecessarily complicate the derivation, we only regard the regularized causal action in the final Theorem 3.4.3 in this way, but otherwise choose a pragmatic approach and bear in mind that all variations are obtained by regarding the corresponding objects as functionals of $\mathrm{P}^\varepsilon_\tau \in \mathcal{D}'(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4, \mathbb{C}^4))$ and subsequently taking derivatives with respect to τ as explained in Definition 3.1.4.

Lemma 3.3.6 (Variations of the Regularized Closed Chain)

Let $A^\varepsilon(x,y)$ be the regularized closed chain as derived in Lemma 3.3.2. Replacing $\mathrm{P}^\varepsilon xy$ by a perturbed version $\mathrm{P}^\varepsilon_\tau xy$, computing the first and second variations δA^ε and $\delta^2 A^\varepsilon$ and decomposing them in the same way as in Lemma 3.3.2 yields

$$\delta A^\varepsilon = \delta A^\varepsilon_{ij}[\gamma^i, \gamma^j] + \delta A^\varepsilon_i \gamma^i + \delta A^\varepsilon_{\mathrm{s}} \tag{3.21a}$$
$$\delta^2 A^\varepsilon = \delta^2 A^\varepsilon_{ij}[\gamma^i, \gamma^j] + \delta^2 A^\varepsilon_i \gamma^i + \delta^2 A^\varepsilon_{\mathrm{s}} \tag{3.21b}$$

Here the component functions $\delta A^\varepsilon_{ij} \in \mathcal{D}'(\mathbb{R}^4, \mathbb{C})$ and $\delta A^\varepsilon_i, \delta A^\varepsilon_{\mathrm{s}} \in \mathcal{D}'(\mathbb{R}^4, \mathbb{R})$ of the first variation are given by

$$\delta A^\varepsilon_{ij} = \frac{1}{2}\big(\delta v^\varepsilon_i \overline{v^\varepsilon_j} + v^\varepsilon_i \overline{\delta v^\varepsilon_j}\big) \tag{3.21a,i}$$
$$\delta A^\varepsilon_i = 2\,\mathrm{Re}\,\big(\delta v^\varepsilon_i \overline{s^\varepsilon} + v^\varepsilon_i \overline{\delta s^\varepsilon}\big) \tag{3.21a,ii}$$
$$\delta A^\varepsilon_{\mathrm{s}} = \mathrm{Re}\,\big(2(\overline{v^i_\varepsilon}\delta v^\varepsilon_i) + 2\overline{s^\varepsilon}\delta s^\varepsilon\big) \tag{3.21a,iii}$$

while at second order we have for $\delta^2 A^\varepsilon_{ij} \in \mathcal{D}'(\mathbb{R}^4, \mathbb{C})$ and $\delta^2 A^\varepsilon_i, \delta^2 A^\varepsilon_{\mathrm{s}} \in \mathcal{D}'(\mathbb{R}^4, \mathbb{R})$ the expressions

$$\delta^2 A^\varepsilon_{ij} = \frac{1}{2}\big(\delta^2 v^\varepsilon_i \overline{v^\varepsilon_j} + v^\varepsilon_i \delta^2\overline{v^\varepsilon_j} + \delta v^\varepsilon_i \overline{\delta v^\varepsilon_j}\big) \tag{3.21b,i}$$
$$\delta^2 A^\varepsilon_i = 2\,\mathrm{Re}\,\big(\delta^2 v^\varepsilon_i \overline{s^\varepsilon} + v^\varepsilon_i \delta^2\overline{s^\varepsilon} + \delta v^\varepsilon_i \overline{\delta s^\varepsilon}\big) \tag{3.21b,ii}$$
$$\delta^2 A^\varepsilon_{\mathrm{s}} = \mathrm{Re}\,\big(2(\overline{v^i_\varepsilon}\delta^2 v^\varepsilon_i) + 2\overline{s^\varepsilon}\delta^2 s^\varepsilon + (\delta v^i_\varepsilon \overline{\delta v^\varepsilon_i}) + \delta s^\varepsilon \overline{\delta s^\varepsilon}\,\big) \tag{3.21b,iii}$$

respectively.[a]

Proof. Inserting the perturbed regularized kernel of the fermionic projector into the expression for the regularized closed chain as given in (3.13), taking the derivative with respect to τ and evaluating at $\tau = 0$ yields

$$\delta A^\varepsilon_{ij} = \frac{\mathrm{d}A^\varepsilon_{\tau,ij}(x,y)}{\mathrm{d}\tau}\bigg|_{\tau=0} = \frac{1}{2}\left(\frac{\mathrm{d}v^\varepsilon_{\tau,i}}{\mathrm{d}\tau}\overline{v^\varepsilon_{\tau,j}} + v^\varepsilon_{\tau,i}\frac{\mathrm{d}\overline{v^\varepsilon_{\tau,j}}}{\mathrm{d}\tau}\right)\bigg|_{\tau=0} = \frac{1}{2}\big(\delta v^\varepsilon_i \overline{v^\varepsilon_j} + v^\varepsilon_i \overline{\delta v^\varepsilon_j}\big)$$

$$\delta A^\varepsilon_i = \frac{\mathrm{d}A^\varepsilon_{\tau,i}(x,y)}{\mathrm{d}\tau}\bigg|_{\tau=0} = 2\,\mathrm{Re}\left(\frac{\mathrm{d}v^\varepsilon_{\tau,i}}{\mathrm{d}\tau}\overline{s^\varepsilon_\tau} + v^\varepsilon_{\tau,i}\frac{\mathrm{d}\overline{s^\varepsilon_\tau}}{\mathrm{d}\tau}\right)\bigg|_{\tau=0} = 2\,\mathrm{Re}\,\big(\delta v^\varepsilon_i \overline{s^\varepsilon} + v^\varepsilon_i \overline{\delta s^\varepsilon}\big)$$

$$\begin{aligned}\delta A^\varepsilon_{\mathrm{s}} = \frac{\mathrm{d}A^\varepsilon_{\tau,\mathrm{s}}(x,y)}{\mathrm{d}\tau}\bigg|_{\tau=0} &= \left(\eta^{ij}\frac{\mathrm{d}v^\varepsilon_{\tau,i}}{\mathrm{d}\tau}\overline{v^\varepsilon_{\tau,j}} + \eta^{ij}v^\varepsilon_{\tau,i}\frac{\mathrm{d}\overline{v^\varepsilon_{\tau,j}}}{\mathrm{d}\tau} + \frac{\mathrm{d}s^\varepsilon_\tau}{\mathrm{d}\tau}\overline{s^\varepsilon_\tau} + s^\varepsilon_\tau\frac{\mathrm{d}\overline{s^\varepsilon_\tau}}{\mathrm{d}\tau}\right)\bigg|_{\tau=0} \\ &= \eta^{ij}\delta v^\varepsilon_i \overline{v^\varepsilon_j} + \eta^{ij} v^\varepsilon_i \overline{\delta v^\varepsilon_i} + \delta s^\varepsilon \overline{s^\varepsilon} + s^\varepsilon \overline{\delta s^\varepsilon} \\ &= 2\,\mathrm{Re}\,\big((\overline{v^i_\varepsilon}\delta v^\varepsilon_i) + \overline{s^\varepsilon}\delta s^\varepsilon\big)\end{aligned}$$

where we have set $v^\varepsilon_{0,i} := v^\varepsilon_i$ and $s^\varepsilon_0 := s^\varepsilon$. Proceeding for the second variations in exactly the same way and expressing everything in terms of first and second variations of the regularized kernel of the fermionic projector by using $\delta^{(n)}(\,\cdot\,) = \frac{1}{n!}\frac{\mathrm{d}^n(\,\cdot\,)_\tau}{\mathrm{d}\tau^n}|_{\tau=0}$ yields

$$\delta^2 A^\varepsilon_{ij} = \frac{1}{2}\cdot\frac{1}{2}\left(\frac{\mathrm{d}^2 v^\varepsilon_{\tau,i}}{\mathrm{d}\tau^2}\overline{v^\varepsilon_{\tau,j}} + v^\varepsilon_{\tau,i}\frac{\mathrm{d}^2\overline{v^\varepsilon_{\tau,j}}}{\mathrm{d}\tau^2} + 2\frac{\mathrm{d}v^\varepsilon_{\tau,i}}{\mathrm{d}\tau}\frac{\mathrm{d}\overline{v^\varepsilon_{\tau,j}}}{\mathrm{d}\tau}\right)\bigg|_{\tau=0} = \frac{1}{2}\big(\delta^2 v^\varepsilon_i \overline{v^\varepsilon_j} + v^\varepsilon_i \delta^2\overline{v^\varepsilon_j} + \delta v^\varepsilon_i \overline{\delta v^\varepsilon_j}\big)$$

$$\delta^2 A_i^\varepsilon = \frac{1}{2}\cdot 2\,\mathrm{Re}\left(\frac{\mathrm{d}^2 v^\varepsilon_{\tau,i}}{\mathrm{d}\tau^2}\overline{s^\varepsilon_\tau} + v^\varepsilon_{\tau,i}\frac{\mathrm{d}^2\overline{s^\varepsilon_\tau}}{\mathrm{d}\tau^2} + 2\frac{\mathrm{d}v^\varepsilon_{\tau,i}}{\mathrm{d}\tau}\frac{\mathrm{d}\overline{s^\varepsilon_\tau}}{\mathrm{d}\tau}\right)\Bigg|_{\tau=0} = 2\,\mathrm{Re}\left(\delta^2 v_i^\varepsilon\overline{s^\varepsilon} + v_i^\varepsilon\delta^2\overline{s^\varepsilon} + \delta v_i^\varepsilon\delta\overline{s^\varepsilon}\right)$$

$$\begin{aligned}\delta^2 A_{\mathrm{s}}^\varepsilon &= \frac{1}{2}\left(\eta^{ij}\frac{\mathrm{d}^2 v^\varepsilon_{\tau,i}}{\mathrm{d}\tau^2}\overline{v^\varepsilon_{\tau,j}} + \eta^{ij}v^\varepsilon_{\tau,i}\frac{\mathrm{d}^2\overline{v^\varepsilon_{\tau,j}}}{\mathrm{d}\tau^2} + \frac{\mathrm{d}^2 s^\varepsilon_\tau}{\mathrm{d}\tau^2}\overline{s^\varepsilon_\tau} + s^\varepsilon_\tau\frac{\mathrm{d}^2\overline{s^\varepsilon_\tau}}{\mathrm{d}\tau^2} + 2\eta^{ij}\frac{\mathrm{d}v^\varepsilon_{\tau,i}}{\mathrm{d}\tau}\frac{\mathrm{d}\overline{v^\varepsilon_{\tau,j}}}{\mathrm{d}\tau} + 2\frac{\mathrm{d}s^\varepsilon_\tau}{\mathrm{d}\tau}\frac{\mathrm{d}\overline{s^\varepsilon_\tau}}{\mathrm{d}\tau}\right)\Bigg|_{\tau=0}\\ &= \left(\eta^{ij}\delta^2 v_i^\varepsilon\overline{v_j^\varepsilon} + \eta^{ij}v_i^\varepsilon\delta^2\overline{v_j^\varepsilon} + \delta^2 s^\varepsilon\overline{s^\varepsilon} + s^\varepsilon\delta^2\overline{s^\varepsilon} + \eta^{ij}\delta v_i^\varepsilon\delta\overline{v_j^\varepsilon} + \delta s^\varepsilon\delta\overline{s^\varepsilon}\right)\\ &= \mathrm{Re}\left(2(\overline{v^i_\varepsilon}\delta^2 v_i^\varepsilon) + 2\overline{s^\varepsilon}\delta^2 s^\varepsilon + (\delta v^i_\varepsilon\delta\overline{v_i^\varepsilon}) + \delta s^\varepsilon\delta\overline{s^\varepsilon}\right)\end{aligned}$$

This concludes the proof. □

[a] For completeness, we remark that we have identified, without explicitly mentioning, $\delta\mathrm{P}^\varepsilon \in \mathrm{L}(\mathbb{R}, \mathcal{D}'(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4,\mathbb{C}^4))) \simeq \mathcal{D}'(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4,\mathbb{C}^4))$ and similarly for the second variation.

Equipped with these intermediate results, we are now ready to derive expressions for the variation of the eigenvalues of the regularized closed chain.

Lemma 3.3.7 (Variation of the Eigenvalues of $A^\varepsilon_\tau(x,y)$)

Let $A^\varepsilon_\tau(x,y)$ be the regularized closed chain as derived in Lemma 3.3.2 with the regularized kernel of the fermionic projector P^ε replaced by a perturbed version $\mathrm{P}^\varepsilon_\tau$. Computing the variation of the corresponding perturbed eigenvalues using Definition 3.1.4 yields

$$\begin{aligned}\delta\lambda^\varepsilon_\pm &= 2\,\mathrm{Re}\left[(\overline{v^i_\varepsilon}\delta v_i^\varepsilon) + \overline{s^\varepsilon}\delta s^\varepsilon\right]\\ &\quad\pm\frac{2}{\sqrt{\mathfrak{D}^\varepsilon}}\,\mathrm{Re}\left[B^\varepsilon(\overline{v^i_\varepsilon}\delta v_i^\varepsilon) - C^\varepsilon(v^i_\varepsilon\delta v_i^\varepsilon) + \left(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\right)\delta s^\varepsilon\right]\end{aligned} \tag{3.22a}$$

and

$$\begin{aligned}\delta^2\lambda^\varepsilon_\pm &= \mathrm{Re}\left[2(\overline{v^i_\varepsilon}\delta^2 v_i^\varepsilon) + 2\overline{s^\varepsilon}\delta^2 s^\varepsilon + (\delta v^i_\varepsilon\delta\overline{v_i^\varepsilon}) + \delta s^\varepsilon\delta\overline{s^\varepsilon}\right]\\ &\quad\pm\frac{1}{\sqrt{\mathfrak{D}^\varepsilon}}\,\mathrm{Re}\Big[2B^\varepsilon(\overline{v^i_\varepsilon}\delta^2 v_i^\varepsilon) - 2C^\varepsilon(v^i_\varepsilon\delta^2 v_i^\varepsilon) + 2\left(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\right)\delta^2 s^\varepsilon\\ &\qquad + 2\left(s^\varepsilon(\overline{v^i_\varepsilon}\delta v_i^\varepsilon) + \overline{s^\varepsilon}(v^i_\varepsilon\delta v_i^\varepsilon)\right)\delta\overline{s^\varepsilon} - (v^i_\varepsilon\delta v_j^\varepsilon)(\overline{v^j_\varepsilon}\delta\overline{v_i^\varepsilon})\\ &\qquad + (v^i_\varepsilon\delta\overline{v_i^\varepsilon})(\overline{v^j_\varepsilon}\delta v_j^\varepsilon) - C^\varepsilon(\delta v^k_\varepsilon\delta v_k^\varepsilon) + B^\varepsilon(\delta v^k_\varepsilon\delta\overline{v_k^\varepsilon})\Big]\\ &\quad\mp\frac{1}{(\mathfrak{D}^\varepsilon)^{3/2}}\,\mathrm{Re}\Big[(C^\varepsilon)^2(v^k_\varepsilon\delta v_k^\varepsilon)^2 - 2B^\varepsilon C^\varepsilon(v^k_\varepsilon\delta v_k^\varepsilon)(\overline{v^k_\varepsilon}\delta v_k^\varepsilon) - 2B^\varepsilon C^\varepsilon(v^k_\varepsilon\delta v_k^\varepsilon)(v^k_\varepsilon\delta\overline{v_k^\varepsilon})\\ &\qquad + (B^\varepsilon)^2(v^k_\varepsilon\delta v_k^\varepsilon)(\overline{v^k_\varepsilon}\delta\overline{v_k^\varepsilon}) + |C^\varepsilon|^2(\overline{v^k_\varepsilon}\delta v_k^\varepsilon)^2 + (B^\varepsilon)^2(\overline{v^k_\varepsilon}\delta v_k^\varepsilon)(v^k_\varepsilon\delta\overline{v_k^\varepsilon})\\ &\qquad - 2C^\varepsilon\left(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\right)(v^k_\varepsilon\delta v_k^\varepsilon)\delta s^\varepsilon + 2C^\varepsilon\left(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon}\overline{s^\varepsilon}\right)(\overline{v^k_\varepsilon}\delta v_k^\varepsilon)\delta s^\varepsilon\\ &\qquad + 2B^\varepsilon\left(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\right)\left((v^k_\varepsilon\delta\overline{v_k^\varepsilon})\delta s^\varepsilon - (v^k_\varepsilon\delta v_k^\varepsilon)\delta\overline{s^\varepsilon}\right)\\ &\qquad + \left(|(v^\varepsilon)^2|^2 - (|v^\varepsilon|^2)^2\right)\left(C^\varepsilon(\delta s^\varepsilon)^2 + B^\varepsilon\delta s^\varepsilon\delta\overline{s^\varepsilon}\right)\Big]\end{aligned} \tag{3.22b}$$

respectively.

Proof. The derivation of the variation of the eigenvalues is complicated by the fact that introducing a perturbation of the regularized closed chain may remove the initial twofold degeneracy of the eigenvalues $\lambda^\varepsilon_\pm(x,y)$. As a consequence, also the spectral projector operators need to be modified as explained by Finster.[11, Sec. 2.6.3] In order to compute the variation of the eigenvalues which traces back to perturbations of the regularized kernel of the fermionic projector, we follow the approach by Kato[73, Ch. 2, § 2] according to which the variation of the eigenvalues at first and second order are given by[a]

$$\delta\lambda^\varepsilon_\pm(x,y) = \frac{1}{2}\,\mathrm{Tr}\left(F^\varepsilon_\pm(x,y)\delta A^\varepsilon(x,y)\right) \tag{3.23a}$$

$$\delta^2\lambda^\varepsilon_\pm(x,y) = \frac{1}{2}\operatorname{Tr}\left(F^\varepsilon_\pm(x,y)\delta^2 A^\varepsilon(x,y) + \frac{F^\varepsilon_\pm(x,y)\delta A^\varepsilon(x,y)F^\varepsilon_\mp(x,y)\delta A^\varepsilon(x,y)}{\lambda^\varepsilon_\pm(x,y)-\lambda^\varepsilon_\mp(x,y)}\right) \tag{3.23b}$$

where the leading factors $\frac{1}{2}$ account for the two-fold degeneracy of the unperturbed eigenvalues and $F^\varepsilon_\pm(x,y)$ denote the unperturbed spectral projectors on the corresponding eigenspaces.

(1) First Variation of the Eigenvalues

We start by inserting the decomposition of the regularized spectral projectors and the variation of the regularized closed chain into bilinear, vector and scalar parts as derived in Lemma 3.3.5 and Lemma 3.3.6. Recalling that traces of an odd number of Dirac matrices vanish identically, (3.23a) reads

$$\begin{aligned}\delta\lambda^\varepsilon_\pm &\overset{(3.23a)}{=} \frac{1}{2}\operatorname{Tr}\Big[F^\varepsilon_{\pm,s}\delta A^\varepsilon_s \mathrm{id}_{\mathbb{C}^4} + F^\varepsilon_{\pm,s}\delta A^\varepsilon_{kl}[\gamma^k,\gamma^l] + F^\varepsilon_{\pm,i}\delta A^\varepsilon_j(x,y)\gamma^i\gamma^j \\ &\qquad + F^\varepsilon_{\pm,ij}\delta A^\varepsilon_{,s}[\gamma^i,\gamma^j] + F^\varepsilon_{\pm,ij}(x,y)\delta A^\varepsilon_{kl}[\gamma^i,\gamma^j][\gamma^k,\gamma^l]\Big] \\ &= \frac{1}{2}\Big[4F^\varepsilon_{\pm,s}\delta A^\varepsilon_s + 4\eta^{ij}F^\varepsilon_{\pm,i}\delta A^\varepsilon_j + F^\varepsilon_{\pm,ij}\delta A^\varepsilon_{kl}\operatorname{Tr}\big([\gamma^i,\gamma^j][\gamma^k,\gamma^l]\big)\Big]\end{aligned}$$

To proceed, we make use of the relation $\operatorname{Tr}\big[[\gamma^i,\gamma^j][\gamma^k,\gamma^l]\big] = 16\big(-\eta^{ik}\eta^{jl}+\eta^{il}\eta^{jk}\big)$ from (B.3c) and insert the explicit expressions for the individual components of the regularized spectral projector and the variation of the regularized closed chain from (3.18) and (3.21), respectively. In this way we arrive at

$$\begin{aligned}\ldots &\underset{(3.21)}{\overset{(3.18)}{=}} \frac{1}{2}\Bigg[2\cdot 2\operatorname{Re}\big((\overline{v^i_\varepsilon}\delta v^\varepsilon_i) + \overline{s^\varepsilon}\delta s^\varepsilon\big) \pm 8\eta^{ij}\frac{\operatorname{Re}\big(v^\varepsilon_i\overline{s^\varepsilon}\big)}{\sqrt{\mathcal{D}^\varepsilon}}\operatorname{Re}\Big(\delta v^\varepsilon_j\overline{s^\varepsilon} + v^\varepsilon_j\overline{\delta s^\varepsilon}\Big) \\ &\qquad \pm 2\big(-\eta^{ik}\eta^{jl}+\eta^{il}\eta^{jk}\big)\frac{v^\varepsilon_i\overline{v^\varepsilon_j}}{\sqrt{\mathcal{D}^\varepsilon}}\Big(\delta v^\varepsilon_k\overline{v^\varepsilon_l} + v^\varepsilon_k\overline{\delta v^\varepsilon_l}\Big)\Bigg]\end{aligned}$$

Spelling out all the products (whereby using $\operatorname{Re}(x)\operatorname{Re}(y) = \frac{1}{2}\operatorname{Re}(xy+\overline{x}y)$ for the second term in the first line), sorting terms according to their power in $\mathcal{D}^\varepsilon$ results in

$$\begin{aligned}\ldots &= 2\operatorname{Re}\Big[(\overline{v^i_\varepsilon}\delta v^\varepsilon_i) + \overline{s^\varepsilon}\delta s^\varepsilon\Big] \\ &\quad \pm \frac{2}{\sqrt{\mathcal{D}^\varepsilon}}\operatorname{Re}\Big[\big((\overline{s^\varepsilon})^2 - (\overline{v^\varepsilon})^2\big)(v^i_\varepsilon\delta v^\varepsilon_i) + \big((v^\varepsilon)^2\overline{s^\varepsilon} + |v^\varepsilon|^2 s^\varepsilon\big)\overline{\delta s^\varepsilon} + \big(|s^\varepsilon|^2 + |v^\varepsilon|^2\big)(\overline{v^i_\varepsilon}\delta v^\varepsilon_i)\Big]\end{aligned}$$

Finally, expressing everything in terms of the functions $B^\varepsilon, C^\varepsilon$ defined in Definition 3.3.3 and using the relation $(\overline{v^\varepsilon})^2 s^\varepsilon + |v^\varepsilon|^2\overline{s^\varepsilon} \underset{(3.15)}{\overset{(3.15)}{=}} B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon$ we end up with the claimed expression

$$\delta\lambda^\varepsilon_\pm \underset{(3.15)}{\overset{(3.15)}{=}} 2\operatorname{Re}\Big[(\overline{v^i_\varepsilon}\delta v^\varepsilon_i) + \overline{s^\varepsilon}\delta s^\varepsilon\Big] \pm \frac{2}{\sqrt{\mathcal{D}^\varepsilon}}\operatorname{Re}\Big[B^\varepsilon(\overline{v^i_\varepsilon}\delta v^\varepsilon_i) - C^\varepsilon(v^i_\varepsilon\delta v^\varepsilon_i) + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta s^\varepsilon\Big]$$

(2) Second Variation of the Eigenvalues

For the evaluation of the second variation we basically proceed in the same way. However, due to the second term in (3.23b) which contains various products involving Dirac matrices and commutators of Dirac matrices, explicit calculations become lengthy and extremely tedious. In order to make the derivation comprehensible for the interested reader, we present the full details in a structured manner in Appendix B: Second Variation of the Eigenvalues of the Regularized Closed Chain.

This concludes the proof. □

[a] Equivalently, these formulas can also be obtained from Finster's discussion.[11, eq. (2.6.5)]

3.4 The Regularized Causal Action

In this final section of the present chapter, we bring together all results from the previous sections to eventually arrive at an expression for the variation of regularized causal action which in turn will serve as the starting point for the following chapter.

3.4.1 Variation of the Regularized Causal Lagrangian

We start by customizing the regularized causal Lagrangian introduced in Definition 2.2.14 to our specific case, namely for regularized kernels of the fermionic projector with vector-scalar structure.

Lemma 3.4.1 (Regularized Causal Lagrangian for P^ε as in Assumption 3.2.2)

Let P^ε be a regularized kernel of the fermionic projector which has vector-scalar structure. Then the regularized causal Lagrangian takes the form

$$\mathcal{L}^\varepsilon(x,y) = \big(\lambda^\varepsilon_+(x,y) - \lambda^\varepsilon_-(x,y)\big)^2 = 4\mathcal{D}^\varepsilon(\xi) \tag{3.24}$$

where $\mathcal{D}^\varepsilon(\xi)$ denotes the regularized discriminant introduced in Definition 3.3.3.

Proof. Inserting the form of the eigenvalues as derived in Lemma 3.3.4 into the definition of the causal Lagrangian, the term $B^\varepsilon(\xi)$ cancels and we immediately arrive at

$$\mathcal{L}^\varepsilon(x,y) = \big(\lambda^\varepsilon_+(x,y) - \lambda^\varepsilon_-(x,y)\big)^2 \overset{(3.16)}{=} \big(2\cdot\mathcal{D}^\varepsilon(\xi)^{1/2}\big)^2 = 4\mathcal{D}^\varepsilon(\xi) \tag{3.25}$$

This concludes the proof. ☐

Based on this expression for the regularized causal Lagrangian, we are now ready to derive its variations at first and second order in perturbation theory.

Lemma 3.4.2 (Variation of the Regularized Causal Lagrangian)

Let $\mathcal{L}^\varepsilon_\tau(x,y)$ be the regularized causal Lagrangian from Lemma 3.4.1 where the eigenvalues $\lambda^\varepsilon_\pm(x,y)$ have been replaced by perturbed versions $\lambda^\varepsilon_{\pm,\tau}(x,y)$. Computing the first and second variations yields

$$\delta\mathcal{L}^\varepsilon = 16\,\mathrm{Re}\Big[B^\varepsilon(\overline{v^i_\varepsilon}\delta v^\varepsilon_i) - C^\varepsilon(v^i_\varepsilon\delta v^\varepsilon_i) + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta s^\varepsilon\Big] \tag{3.26a}$$

and

$$\begin{aligned}\delta^2\mathcal{L}^\varepsilon = 8\,\mathrm{Re}\Big[&2B^\varepsilon(\overline{v^i_\varepsilon}\delta^2 v^\varepsilon_i) - 2C^\varepsilon(v^i_\varepsilon\delta^2 v^\varepsilon_i) + 2\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta^2 s^\varepsilon \\ &+ 2\overline{s^\varepsilon}(\overline{v^i_\varepsilon}\delta v^\varepsilon_i)\delta s^\varepsilon + 4\overline{s^\varepsilon}(v^i_\varepsilon\delta v^\varepsilon_i)\overline{\delta s^\varepsilon} + 2\overline{s^\varepsilon}(v^i_\varepsilon\overline{\delta v^\varepsilon_i})\delta s^\varepsilon \\ &+ (v^i_\varepsilon\overline{\delta v^\varepsilon_i})(\overline{v^j_\varepsilon}\delta v^\varepsilon_j) - 2(v^i_\varepsilon\delta v^\varepsilon_i)(\overline{v^i_\varepsilon}\overline{\delta v^\varepsilon_i}) + (\overline{v^i_\varepsilon}\delta v^\varepsilon_i)^2 \\ &- C^\varepsilon(\delta v^k_\varepsilon\delta v^\varepsilon_k) + B^\varepsilon(\delta v^k_\varepsilon\overline{\delta v^\varepsilon_k}) + (\overline{v^\varepsilon})^2(\delta s^\varepsilon)^2 + |v^\varepsilon|^2\delta s^\varepsilon\overline{\delta s^\varepsilon}\Big]\end{aligned} \tag{3.26b}$$

respectively.

Proof. In order to derive the claimed expressions for the variation of the regularized causal Lagrangian, we recall that the regularized causal Lagrangian is proportional to the square of the difference of the eigenvalues of the regularized closed chain. Perturbing the eigenvalues and taking derivatives with respect to τ yields

$$\begin{aligned}
\delta\mathcal{L}^\varepsilon &= \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}\tau}\left(\lambda^\varepsilon_{+,\tau} - \lambda^\varepsilon_{-,\tau}\right)^2\Big|_{\tau=0} \\
&= 2\big(\lambda^\varepsilon_{+,\tau} - \lambda^\varepsilon_{-,\tau}\big)\left(\frac{\mathrm{d}\lambda^\varepsilon_+}{\mathrm{d}\tau} - \frac{\mathrm{d}\lambda^\varepsilon_-}{\mathrm{d}\tau}\right)\bigg|_{\tau=0} \\
&= 2\big(\lambda^\varepsilon_+ - \lambda^\varepsilon_-\big)\big(\delta\lambda^\varepsilon_+ - \delta\lambda^\varepsilon_-\big)
\end{aligned} \tag{3.27}$$

For the second variation we analogously find

$$\begin{aligned}
\delta^2\mathcal{L}^\varepsilon &= \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}\left(\lambda^\varepsilon_{+,\tau} - \lambda^\varepsilon_{-,\tau}\right)^2\Big|_{\tau=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}\tau}\left[\big(\lambda^\varepsilon_{+,\tau} - \lambda^\varepsilon_{-,\tau}\big)\left(\frac{\mathrm{d}\lambda^\varepsilon_{+,\tau}}{\mathrm{d}\tau} - \frac{\mathrm{d}\lambda^\varepsilon_{-,\tau}}{\mathrm{d}\tau}\right)\right]\bigg|_{\tau=0} \\
&= \left(\frac{\mathrm{d}\lambda^\varepsilon_+}{\mathrm{d}\tau} - \frac{\mathrm{d}\lambda^\varepsilon_-}{\mathrm{d}\tau}\right)^2 + \big(\lambda^\varepsilon_+ - \lambda^\varepsilon_-\big)\left(\frac{\mathrm{d}^2\lambda^\varepsilon_+}{\mathrm{d}\tau^2} - \frac{\mathrm{d}^2\lambda^\varepsilon_-}{\mathrm{d}\tau^2}\right) \\
&= \big(\delta\lambda^\varepsilon_+ - \delta\lambda^\varepsilon_-\big)^2 + 2\big(\lambda^\varepsilon_+ - \lambda^\varepsilon_-\big)\big(\delta^2\lambda^\varepsilon_+ - \delta^2\lambda^\varepsilon_-\big)
\end{aligned} \tag{3.28}$$

where in the last step we used the relation $\delta^2\lambda^\varepsilon_\pm = \frac{1}{2}\frac{\mathrm{d}^2\lambda^\varepsilon_{\pm,\tau}}{\mathrm{d}\tau^2}\big|_{\tau=0}$. To arrive at the claimed expressions, it remains to insert the formulas for $\delta\lambda^\varepsilon_\pm$ and $\delta^2\lambda^\varepsilon_\pm$ from (3.22a) and (3.22b), respectively, along with $\lambda^\varepsilon_+ - \lambda^\varepsilon_- = 2\sqrt{\mathcal{D}^\varepsilon}$. For the first variation of the regularized causal Lagrangian we obtain in this way

$$\begin{aligned}
\delta\mathcal{L}^\varepsilon &\overset{(3.27)}{\underset{(3.22a)}{=}} 2\cdot 2\sqrt{\mathcal{D}^\varepsilon}\cdot\frac{4}{\sqrt{\mathcal{D}^\varepsilon}}\,\mathrm{Re}\Big[B^\varepsilon(\overline{v^i_\varepsilon}\delta v^\varepsilon_i) - C^\varepsilon(v^i_\varepsilon\delta v^\varepsilon_i) + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta s^\varepsilon\Big] \\
&= 16\,\mathrm{Re}\Big[B^\varepsilon(\overline{v^i_\varepsilon}\delta v^\varepsilon_i) - C^\varepsilon(v^i_\varepsilon\delta v^\varepsilon_i) + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta s^\varepsilon\Big]
\end{aligned} \tag{3.29}$$

where the first term in (3.22a) drops out and only the term proportional to $(\mathcal{D}^\varepsilon)^{-1/2}$ remains. For the second variation the procedure is basically the same, though slightly more involved due to the necessity to compute squares of differences which involve several terms. Inserting (3.22a) and (3.22b) into (3.28) yields

$$\begin{aligned}
\delta^2\mathcal{L}^\varepsilon \overset{(3.22a)}{\underset{(3.22b)}{=}} &\left(2\cdot\frac{2}{\sqrt{\mathcal{D}^\varepsilon}}\,\mathrm{Re}\Big[B^\varepsilon(\overline{v^i_\varepsilon}\delta v^\varepsilon_i) - C^\varepsilon(v^i_\varepsilon\delta v^\varepsilon_i) + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta s^\varepsilon\Big]\right)^2 \\
&+ 4\sqrt{\mathcal{D}^\varepsilon}\cdot\Bigg(\frac{1}{\sqrt{\mathcal{D}^\varepsilon}}\,\mathrm{Re}\Big[2B^\varepsilon(\overline{v^i_\varepsilon}\delta^2 v^\varepsilon_i) - 2C^\varepsilon(v^i_\varepsilon\delta^2 v^\varepsilon_i) + 2\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta^2 s^\varepsilon \\
&\qquad + 2\big(s^\varepsilon(\overline{v^i_\varepsilon}\delta v^\varepsilon_i) + \overline{s^\varepsilon}(v^i_\varepsilon\delta v^\varepsilon_i)\big)\overline{\delta s^\varepsilon} - (v^i_\varepsilon\delta v^\varepsilon_j)(\overline{v^i_\varepsilon}\overline{\delta v^\varepsilon_i}) \\
&\qquad + (v^i_\varepsilon\overline{\delta v^\varepsilon_i})(\overline{v^j_\varepsilon}\delta v^\varepsilon_j) - C^\varepsilon(\delta v^k_\varepsilon\delta v^\varepsilon_k) + B^\varepsilon(\delta v^k_\varepsilon\overline{\delta v^\varepsilon_k})\Big] \\
&- \frac{2}{(\mathcal{D}^\varepsilon)^{3/2}}\,\mathrm{Re}\Big[(C^\varepsilon)^2(v^k_\varepsilon\delta v^\varepsilon_k)^2 - 2B^\varepsilon C^\varepsilon(v^k_\varepsilon\delta v^\varepsilon_k)(\overline{v^k_\varepsilon}\delta v^\varepsilon_k) - 2B^\varepsilon C^\varepsilon(v^k_\varepsilon\delta v^\varepsilon_k)(v^k_\varepsilon\overline{\delta v^\varepsilon_k}) \\
&\qquad + (B^\varepsilon)^2(v^k_\varepsilon\delta v^\varepsilon_k)(\overline{v^k_\varepsilon}\overline{\delta v^\varepsilon_k}) + C^\varepsilon\overline{C^\varepsilon}(\overline{v^k_\varepsilon}\delta v^\varepsilon_k)^2 + (B^\varepsilon)^2(\overline{v^k_\varepsilon}\delta v^\varepsilon_k)(v^k_\varepsilon\overline{\delta v^\varepsilon_k}) \\
&\qquad - 2C^\varepsilon\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)(v^k_\varepsilon\delta v^\varepsilon_k)\delta s^\varepsilon + 2C^\varepsilon\big(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon}\overline{s^\varepsilon}\big)(\overline{v^k_\varepsilon}\delta v^\varepsilon_k)\delta s^\varepsilon \\
&\qquad + 2B^\varepsilon\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)(v^k_\varepsilon\overline{\delta v^\varepsilon_k})\delta s^\varepsilon - 2B^\varepsilon\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)(v^k_\varepsilon\delta v^\varepsilon_k)\overline{\delta s^\varepsilon} \\
&\qquad + C^\varepsilon\big(|(v^\varepsilon)^2|^2 - (|v^\varepsilon|^2)^2\big)(\delta s^\varepsilon)^2 + B^\varepsilon\big(|(v^\varepsilon)^2|^2 - (|v^\varepsilon|^2)^2\big)\delta s^\varepsilon\overline{\delta s^\varepsilon}\Big]\Bigg)
\end{aligned}$$

Making use of the relation $(\mathrm{Re}(x))^2 = \frac{1}{2}\mathrm{Re}(|x|^2 + x^2)$ and rearranging terms yields

$$\begin{aligned}
\ldots = 8\,\mathrm{Re}\Big[&2B^\varepsilon(\overline{v^i_\varepsilon}\delta^2 v^\varepsilon_i) - 2C^\varepsilon(v^i_\varepsilon\delta^2 v^\varepsilon_i) + 2\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta^2 s^\varepsilon \\
&+ 2\big(s^\varepsilon(\overline{v^i_\varepsilon}\delta v^\varepsilon_i) + \overline{s^\varepsilon}(v^i_\varepsilon\delta v^\varepsilon_i)\big)\overline{\delta s^\varepsilon} - (v^i_\varepsilon\delta v^\varepsilon_j)(\overline{v^i_\varepsilon}\overline{\delta v^\varepsilon_i})
\end{aligned}$$

$$
\begin{aligned}
&\qquad + (v^i_\varepsilon \delta\overline{v^\varepsilon_i})(\overline{v^j_\varepsilon}\delta v^\varepsilon_j) - C^\varepsilon(\delta v^k_\varepsilon \delta v^\varepsilon_k) + B^\varepsilon(\delta v^k_\varepsilon \delta\overline{v^\varepsilon_k})\Big] \\
&+ \frac{8}{\mathcal{D}^\varepsilon}\,\mathrm{Re}\Big[(C^\varepsilon)^2 \cancelto{(1)}{(v^i_\varepsilon \delta v^\varepsilon_i)^2} - 2B^\varepsilon C^\varepsilon \cancelto{(2)}{(\overline{v^i_\varepsilon}\delta v^\varepsilon_i)(v^i_\varepsilon \delta v^\varepsilon_i)} - 2B^\varepsilon C^\varepsilon \cancelto{(3)}{(v^i_\varepsilon \delta\overline{v^\varepsilon_i})(v^i_\varepsilon \delta v^\varepsilon_i)} \\
&\qquad + C^\varepsilon\overline{C^\varepsilon}(v^i_\varepsilon \delta v^\varepsilon_i)(\overline{v^i_\varepsilon}\delta\overline{v^\varepsilon_i}) + (B^\varepsilon)^2(\overline{v^i_\varepsilon}\delta v^\varepsilon_i)^2 + (B^\varepsilon)^2 \cancelto{(4)}{(\overline{v^i_\varepsilon}\delta v^\varepsilon_i)(\overline{v^i_\varepsilon}\delta v^\varepsilon_i)} \\
&\qquad - 2C^\varepsilon\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\cancelto{(5)}{(v^i_\varepsilon \delta v^\varepsilon_i)\delta s^\varepsilon} + 2B^\varepsilon\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)(\overline{v^i_\varepsilon}\delta v^\varepsilon_i)\delta s^\varepsilon \\
&\qquad + 2B^\varepsilon\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\cancelto{(6)}{(v^i_\varepsilon \delta\overline{v^\varepsilon_i})\delta s^\varepsilon} - 2C^\varepsilon\big(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon}\,\overline{s^\varepsilon}\big)(v^i_\varepsilon \delta v^\varepsilon_i)\delta\overline{s^\varepsilon} \\
&\qquad\qquad + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)^2(\delta s^\varepsilon)^2 + \big|\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta s^\varepsilon\big|^2\Big] \\
&- \frac{8}{\mathcal{D}^\varepsilon}\,\mathrm{Re}\Big[(C^\varepsilon)^2 \cancelto{\text{cancels (1)}}{(v^k_\varepsilon \delta v^\varepsilon_k)^2} - 2B^\varepsilon C^\varepsilon \cancelto{\text{cancels (2)}}{(v^k_\varepsilon \delta v^\varepsilon_k)(\overline{v^k_\varepsilon}\delta v^\varepsilon_k)} - 2B^\varepsilon C^\varepsilon \cancelto{\text{cancels (3)}}{(v^k_\varepsilon \delta v^\varepsilon_k)(v^k_\varepsilon \delta v^\varepsilon_k)} \\
&\qquad + (B^\varepsilon)^2(v^k_\varepsilon \delta v^\varepsilon_k)(\overline{v^k_\varepsilon}\delta\overline{v^\varepsilon_k}) + C^\varepsilon\overline{C^\varepsilon}(\overline{v^k_\varepsilon}\delta v^\varepsilon_k)^2 + (B^\varepsilon)^2 \cancelto{\text{cancels (4)}}{(\overline{v^k_\varepsilon}\delta v^\varepsilon_k)(v^k_\varepsilon \delta v^\varepsilon_k)} \\
&\qquad - 2C^\varepsilon\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\cancelto{\text{cancels (5)}}{(v^k_\varepsilon \delta v^\varepsilon_k)\delta s^\varepsilon} + 2C^\varepsilon\big(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon}\,\overline{s^\varepsilon}\big)(\overline{v^k_\varepsilon}\delta v^\varepsilon_k)\delta s^\varepsilon \\
&\qquad + 2B^\varepsilon\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\cancelto{\text{cancels (6)}}{(v^k_\varepsilon \delta\overline{v^\varepsilon_k})\delta s^\varepsilon} - 2B^\varepsilon\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)(v^k_\varepsilon \delta v^\varepsilon_k)\delta\overline{s^\varepsilon} \\
&\qquad + C^\varepsilon\big(|(v^\varepsilon)^2|^2 - (|v^\varepsilon|^2)^2\big)(\delta s^\varepsilon)^2 + B^\varepsilon\big(|(v^\varepsilon)^2|^2 - (|v^\varepsilon|^2)^2\big)\delta s^\varepsilon\delta\overline{s^\varepsilon}\Big] \\
&= 8\,\mathrm{Re}\Big[2B^\varepsilon(\overline{v^i_\varepsilon}\delta^2 v^\varepsilon_i) - 2C^\varepsilon(v^i_\varepsilon\delta^2 v^\varepsilon_i) + 2\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta^2 s^\varepsilon \\
&\qquad + 2\big(s^\varepsilon(\overline{v^i_\varepsilon}\delta v^\varepsilon_i) + \overline{s^\varepsilon}(v^i_\varepsilon\delta v^\varepsilon_i)\big)\delta\overline{s^\varepsilon} - (v^i_\varepsilon\delta v^\varepsilon_j)(\overline{v^i_\varepsilon}\delta\overline{v^\varepsilon_i}) \\
&\qquad + (v^i_\varepsilon \delta\overline{v^\varepsilon_i})(\overline{v^j_\varepsilon}\delta v^\varepsilon_j) - C^\varepsilon(\delta v^k_\varepsilon \delta v^\varepsilon_k) + B^\varepsilon(\delta v^k_\varepsilon \delta\overline{v^\varepsilon_k})\Big] \\
&+ \frac{8}{\mathcal{D}^\varepsilon}\,\mathrm{Re}\Big[-\mathcal{D}^\varepsilon(v^i_\varepsilon\delta v^\varepsilon_i)(\overline{v^i_\varepsilon}\delta\overline{v^\varepsilon_i}) + \mathcal{D}^\varepsilon(\overline{v^i_\varepsilon}\delta v^\varepsilon_i)^2 \\
&\qquad + 2\mathcal{D}^\varepsilon\overline{s^\varepsilon}(\overline{v^i_\varepsilon}\delta v^\varepsilon_i)\delta s^\varepsilon + 2\mathcal{D}^\varepsilon\overline{s^\varepsilon}(v^i_\varepsilon\delta v^\varepsilon_i)\delta\overline{s^\varepsilon} \\
&\qquad\qquad + \mathcal{D}^\varepsilon(\overline{v^\varepsilon})^2(\delta s^\varepsilon)^2 + \mathcal{D}^\varepsilon|v^\varepsilon|^2\delta s^\varepsilon\delta\overline{s^\varepsilon}\Big]
\end{aligned}
$$

Finally, cancelling terms and combing the remaining ones results in

$$
\begin{aligned}
\delta^2\mathcal{L}^\varepsilon = 8\,\mathrm{Re}\Big[&2B^\varepsilon(\overline{v^i_\varepsilon}\delta^2 v^\varepsilon_i) - 2C^\varepsilon(v^i_\varepsilon\delta^2 v^\varepsilon_i) + 2\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta^2 s^\varepsilon \\
&+ 2\overline{s^\varepsilon}(\overline{v^i_\varepsilon}\delta v^\varepsilon_i)\delta s^\varepsilon + 4\overline{s^\varepsilon}(v^i_\varepsilon\delta v^\varepsilon_i)\delta\overline{s^\varepsilon} + 2\overline{s^\varepsilon}(v^i_\varepsilon\delta\overline{v^\varepsilon_i})\delta s^\varepsilon \\
&+ (v^i_\varepsilon\delta\overline{v^\varepsilon_i})(\overline{v^j_\varepsilon}\delta v^\varepsilon_j) - 2(v^i_\varepsilon\delta v^\varepsilon_i)(\overline{v^i_\varepsilon}\delta\overline{v^\varepsilon_i}) + (\overline{v^i_\varepsilon}\delta v^\varepsilon_i)^2 \\
&- C^\varepsilon(\delta v^k_\varepsilon\delta v^\varepsilon_k) + B^\varepsilon(\delta v^k_\varepsilon\delta\overline{v^\varepsilon_k}) + (\overline{v^\varepsilon})^2(\delta s^\varepsilon)^2 + |v^\varepsilon|^2\delta s^\varepsilon\delta\overline{s^\varepsilon}\Big] \qquad (3.30)
\end{aligned}
$$

This concludes the proof. □

3.4.2 Variation of the Regularized Causal Action

With the expression for the variation of the regularized causal Lagrangian at first and second order at hand, we are finally in the position to derive the corresponding variation of the regularized causal action. In contrast with the above derivations, however, we restrict our considerations to the homogeneous case introduced in Subsection 2.3.3.

Theorem 3.4.3 (First and Second Variation of the Regularized Causal Action)

Let $\mathcal{L}^\varepsilon_{\mathrm{h}} : \mathbb{R}^4 \to \mathbb{R}^+_0$ as well as $\mathcal{S}^\varepsilon_{\mathrm{h}}$ be the homogeneous regularized causal Lagrangian and the homogeneous regularized causal action as introduced in Definition 2.3.5. Furthermore, we assume that $\mathrm{P}_0^\varepsilon \in C^\infty(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4,\mathbb{C}^4))$ is a spherically-symmetric minimizer of $\mathcal{S}_\mathrm{h}^\varepsilon$. Then the first and second variation of the regularized causal action arising from an anisotropically deformed $\mathrm{P}_\tau^\varepsilon \in \mathcal{D}'(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4,\mathbb{C}^4))$ (for $\tau \in (0,\tau_\mathrm{max})$ with $\tau_\mathrm{max} > 0$) around P_0^ε are given by

$$\delta\mathcal{S}_\mathrm{h}^\varepsilon = \int_\mathbb{R} \mathrm{d}\xi^0 \int_{S^2} \mathrm{d}\Omega_\xi \int_0^{R_\mathrm{max}^\varepsilon(\xi^0)} \mathrm{d}r\ r^2 \delta\mathcal{L}_\mathrm{h}^\varepsilon(\xi) \tag{3.31a}$$

$$\delta^2\mathcal{S}_\mathrm{h}^\varepsilon = \int_\mathbb{R} \mathrm{d}\xi^0 \int_{S^2} \mathrm{d}\Omega_\xi \left[\int_0^{R_\mathrm{max}^\varepsilon(\xi^0)} \mathrm{d}r\ r^2 \delta^2\mathcal{L}_\mathrm{h}^\varepsilon(\xi) - \frac{1}{2}\left(r^2 \frac{\delta\mathcal{L}_\mathrm{h}^\varepsilon(\xi)^2}{\partial_r \mathcal{L}_\mathrm{h}^\varepsilon(\xi)} \right)\bigg|_{r=R_\mathrm{max}^\varepsilon(\xi^0)} \right] \tag{3.31b}$$

where $R_\mathrm{max}^\varepsilon : \mathbb{R} \to \mathbb{R}_0^+$ denotes the spherically-symmetric demarcation function corresponding to P_0^ε.

Proof. Before we start with the actual derivation, we shall first establish the connection with Subsection 2.2.4: The homogeneous analogue $\Sigma_\mathrm{h} : C^\infty(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4,\mathbb{C}^4)) \to \mathbb{R}_0^+$ of the causal action evaluation operator associates to a given homogeneous regularized kernel of the fermionic projector P^ε the homogeneous regularized causal action $\mathcal{S}_\mathrm{h}^\varepsilon$. Now, in order to be able to compute variations of Σ_h in the sense of Definition 3.1.4, we have to regard Σ_h as a functional on the space $\mathcal{D}'(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4,\mathbb{C}^4))$ of tempered distributions[a] and evaluate it for some $\mathrm{P}_\tau^\varepsilon \in \mathcal{D}'(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4,\mathbb{C}^4))$ which arises from the minimizer P_0^ε by slightly deforming the regularization.

As a consequence of this deformation, not only the regularized closed chain and its eigenvalues (see Lemma 3.3.7) and thus also the regularized causal Lagrangian (see Lemma 3.4.2) vary, but also the region $\mathcal{R}^\varepsilon$ is affected. More specifically, for an anisotropic deformation, the initially spherically-symmetric demarcation function acquires an angular dependence.

To analyze the effect of the deformation of the regularization on $\mathcal{S}_\mathrm{h}^\varepsilon$ at first and second order in τ, we have to determine the first and second variations $\delta\Sigma_\mathrm{h}$ and $\delta^2\Sigma_\mathrm{h}$ of Σ_h at P_0^ε in the sense of Definition 3.1.4.

(1) First Variation of the Homogeneous Regularized Causal Action

To derive the first variation $\delta\Sigma_\mathrm{h}$, we evaluate Σ_h at $\mathrm{P}_\tau^\varepsilon$ which basically amounts to replacing $\mathcal{L}_\mathrm{h}^\varepsilon$ by $\mathcal{L}_{\mathrm{h},\tau}^\varepsilon$ in (2.41). Due to the fact that $\mathcal{L}_{\mathrm{h},\tau}^\varepsilon(\xi)$ vanishes for $\xi \in \mathbb{R}^4 \setminus \mathcal{R}_\tau^\varepsilon$, we can furthermore replace the domain of integration $\mathbb{R}^4$ by $\mathcal{R}_\tau^\varepsilon$. Now, by taking the derivative of this expression with respect to the parameter τ and evaluating at $\tau = 0$ gives exactly the first variation $\delta\Sigma_\mathrm{h}$

$$\big(\delta\Sigma_\mathrm{h}(\mathrm{P}_0^\varepsilon)\big)(\delta\mathrm{P}^\varepsilon) = $$
$$= \frac{\mathrm{d}}{\mathrm{d}\tau}\left[\int_{\mathcal{R}_\tau^\varepsilon} \mathrm{d}^4\xi\, \mathcal{L}_{\mathrm{h},\tau}^\varepsilon(\xi) \right]\Bigg|_{\tau=0} = \frac{\mathrm{d}}{\mathrm{d}\tau}\left[\int_\mathbb{R} \mathrm{d}\xi^0 \int_{S^2} \mathrm{d}\Omega_\xi \int_0^{R_{\mathrm{max},\tau}^\varepsilon(\xi^0,\theta,\varphi)} \mathrm{d}r\ r^2 \mathcal{L}_{\mathrm{h},\tau}^\varepsilon(\xi) \right]\Bigg|_{\tau=0}$$

Suppressing arguments and carrying out the derivative by exploiting Leibniz's integral rule for differentiation under the integral sign yields

$$\cdots = \int_\mathbb{R} \mathrm{d}\xi^0 \int_{S^2} \mathrm{d}\Omega_\xi \left[\int_0^{R_{\mathrm{max},\tau}^\varepsilon} \mathrm{d}r\ r^2 \frac{\mathrm{d}\mathcal{L}_{\mathrm{h},\tau}^\varepsilon}{\mathrm{d}\tau} + \left(r^2 \mathcal{L}_{\mathrm{h},\tau}^\varepsilon \right)\Big|_{r=R_{\mathrm{max},\tau}^\varepsilon} \frac{\mathrm{d}R_{\mathrm{max},\tau}^\varepsilon}{\mathrm{d}\tau} \right]\Bigg|_{\tau=0} \tag{3.32}$$

Using that $R_{\mathrm{max},\tau}^\varepsilon$ and $\mathcal{L}_{\mathrm{h},\tau}^\varepsilon$ reduce to $R_\mathrm{max}^\varepsilon$ and $\mathcal{L}_\mathrm{h}^\varepsilon$ in the limit $\tau \to 0$ and employing the definition of the demarcation function, we conclude that the second term vanishes identically.

We thus end up with

$$\big(\delta\Sigma_{\mathrm{h}}(\mathrm{P}^\varepsilon_0)\big)(\delta\mathrm{P}^\varepsilon) = \int\limits_{\mathbb{R}} \mathrm{d}\xi^0 \int\limits_{S^2} \mathrm{d}\Omega_\xi \int\limits_0^{R^\varepsilon_{\max}(\xi^0)} \mathrm{d}r\ r^2 \delta\mathcal{L}^\varepsilon_{\mathrm{h}}(\xi) \tag{3.33}$$

where the variation $\delta\mathcal{L}^\varepsilon_{\mathrm{h}}$ must be understood as a function of $\delta\mathrm{P}^\varepsilon$ as given in (3.26a). To arrive at a more suggestive notation, we will from now on replace $\big(\delta\Sigma_{\mathrm{h}}(\mathrm{P}^\varepsilon_0)\big)(\delta\mathrm{P}^\varepsilon)$ by $\delta\mathcal{S}^\varepsilon_{\mathrm{h}}$.

(2) Second Variation of the Homogeneous Regularized Causal Action

For the derivation of the second variation $\delta^2\Sigma_{\mathrm{h}}$ we proceed in the same way as above: Starting from the same initial expression, suppressing arguments and taking second derivatives with respect to τ yields

$$\begin{aligned}
&\big(\delta^2\Sigma_{\mathrm{h}}(\mathrm{P}^\varepsilon_0)\big)(\delta\mathrm{P}^\varepsilon, \delta^2\mathrm{P}^\varepsilon) = \\
&\quad = \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}\left[\int\limits_{\mathbb{R}} \mathrm{d}\xi^0 \int\limits_{S^2} \mathrm{d}\Omega_\xi \int\limits_0^{R^\varepsilon_{\max,\tau}(\xi^0,\theta,\varphi)} \mathrm{d}r\ r^2 \mathcal{L}^\varepsilon_{\mathrm{h},\tau}(\xi)\right]\Bigg|_{\tau=0} \\
&\quad \overset{(3.32)}{=} \frac{1}{2}\int\limits_{\mathbb{R}} \mathrm{d}\xi^0 \int\limits_{S^2} \mathrm{d}\Omega_\xi \left[\int\limits_0^{R^\varepsilon_{\max,\tau}} \mathrm{d}r\ r^2 \frac{\mathrm{d}^2\mathcal{L}^\varepsilon_{\mathrm{h},\tau}}{\mathrm{d}\tau^2} + \left(r^2\frac{\mathrm{d}\mathcal{L}^\varepsilon_{\mathrm{h},\tau}}{\mathrm{d}\tau}\right)\bigg|_{r=R^\varepsilon_{\max,\tau}} \frac{\mathrm{d}R^\varepsilon_{\max,\tau}}{\mathrm{d}\tau}\right. \\
&\qquad\qquad \left. + \frac{\mathrm{d}}{\mathrm{d}\tau}\left(\left(r^2\mathcal{L}^\varepsilon_{\mathrm{h},\tau}\right)\Big|_{r=R^\varepsilon_{\max,\tau}} \frac{\mathrm{d}R^\varepsilon_{\max,\tau}}{\mathrm{d}\tau}\right)\right]\Bigg|_{\tau=0}
\end{aligned}$$

Spelling out the derivative in the last term and combining the resulting terms with the last term in the first line yields

$$\begin{aligned}
\cdots = \frac{1}{2}\int\limits_{\mathbb{R}} \mathrm{d}\xi^0 \int\limits_{S^2} \mathrm{d}\Omega_\xi &\left[\int\limits_0^{R^\varepsilon_{\max,\tau}} \mathrm{d}r\ r^2 \frac{\mathrm{d}^2\mathcal{L}^\varepsilon_{\mathrm{h},\tau}}{\mathrm{d}\tau^2} + \left(2r^2\frac{\mathrm{d}\mathcal{L}^\varepsilon_{\mathrm{h},\tau}}{\mathrm{d}\tau}\frac{\mathrm{d}R^\varepsilon_{\max,\tau}}{\mathrm{d}\tau} + r^2\frac{\partial\mathcal{L}^\varepsilon_{\mathrm{h},\tau}}{\partial r}\left(\frac{\mathrm{d}R^\varepsilon_{\max,\tau}}{\mathrm{d}\tau}\right)^2\right.\right. \\
&\qquad \left.\left. + \frac{\mathcal{L}^\varepsilon_{\mathrm{h},\tau}}{3}\frac{\mathrm{d}^2(R^\varepsilon_{\max,\tau})^3}{\mathrm{d}\tau^2}\right)\bigg|_{r=R^\varepsilon_{\max,\tau}}\right]\Bigg|_{\tau=0}
\end{aligned}$$

Note that in order to arrive at this result we have used that $\mathcal{L}^\varepsilon_{\mathrm{h},\tau}(\xi)|_{r=R^\varepsilon_{\max,\tau}}$ depends on the parameter τ in two different ways: On the one hand, the parameter τ represents the change in the function $\mathcal{L}^\varepsilon_{\mathrm{h}}$ itself, which traces back to the replacement $\mathrm{P}^\varepsilon_0 \to \mathrm{P}^\varepsilon_\tau$ and leads to the *intrinsic change* denoted by $\frac{\mathrm{d}\mathcal{L}^\varepsilon_{\mathrm{h},\tau}}{\mathrm{d}\tau}\big|_{\tau=0}$. On the other hand, however, also the argument $\xi = (\xi^0, R^\varepsilon_{\max,\tau}, \theta, \varphi)$ depends on τ which leads to the appearance of partial derivatives of $\mathcal{L}^\varepsilon_{\mathrm{h},\tau}$ with respect to the radial variable r. By evaluating the expression at $\tau = 0$ and using that the regularized causal Lagrangian vanishes upon evaluation at $r = R^\varepsilon_{\max}(\xi^0)$, the term in the second line vanishes and we are left with

$$\begin{aligned}
&\big(\delta^2\Sigma_{\mathrm{h}}(\mathrm{P}^\varepsilon_0)\big)(\delta\mathrm{P}^\varepsilon, \delta^2\mathrm{P}^\varepsilon) = \\
&\quad = \frac{1}{2}\int\limits_{\mathbb{R}} \mathrm{d}\xi^0 \int\limits_{S^2} \mathrm{d}\Omega_\xi \left[\int\limits_0^{R^\varepsilon_{\max}(\xi^0)} \mathrm{d}r\ r^2 \frac{\mathrm{d}^2\mathcal{L}^\varepsilon_{\mathrm{h},\tau}}{\mathrm{d}\tau^2}\bigg|_{\tau=0}\right. \\
&\qquad\qquad \left. + \left(2r^2\frac{\mathrm{d}\mathcal{L}^\varepsilon_{\mathrm{h},\tau}}{\mathrm{d}\tau}\frac{\mathrm{d}R^\varepsilon_{\max,\tau}}{\mathrm{d}\tau} + r^2\frac{\partial\mathcal{L}^\varepsilon_{\mathrm{h},\tau}}{\partial r}\left(\frac{\mathrm{d}R^\varepsilon_{\max,\tau}}{\mathrm{d}\tau}\right)^2\right)\bigg|_{r=R^\varepsilon_{\max,\tau}}\right]\Bigg|_{\tau=0}
\end{aligned}$$

In contrast with the first variation calculated above, the deformation of the domain of integration does give a contribution at second order. The deformation of the demarcation function compared with $R^\varepsilon_{\max}$ is encoded in the derivatives of $R^\varepsilon_{\max,\tau}$ with respect to τ. Due to the fact that the demarcation function is defined in terms of the regularized causal Lagrangian, we can trade in its derivatives for derivatives of the regularized causal Lagrangian. Considering the defining conditions for the deformed and undeformed demarcation function

$$0 = \mathcal{L}^\varepsilon_{\mathrm{h}}(\xi)\big|_{r=R^\varepsilon_{\max}(\xi^0)} \qquad \text{and} \qquad 0 = \mathcal{L}^\varepsilon_{\mathrm{h},\tau}(\xi)\big|_{r=R^\varepsilon_{\max,\tau}(\xi^0,\theta,\varphi)}$$

and expanding their difference in a Taylor series in the parameter τ up to first order yields

$$\begin{aligned} 0 &= \mathcal{L}^\varepsilon_{\mathrm{h},\tau}(\xi)\big|_{r=R^\varepsilon_{\max,\tau}(\xi^0,\theta,\varphi)} - \mathcal{L}^\varepsilon(\xi)\big|_{r=R^\varepsilon_{\max}(\xi^0)} \\ &= \mathcal{L}^\varepsilon_{\mathrm{h},\tau}\big(\xi^0, R^\varepsilon_{\max,\tau}(\xi^0,\theta,\varphi),\theta,\varphi\big) - \mathcal{L}^\varepsilon(\xi)\big|_{r=R^\varepsilon_{\max}(\xi^0)} \\ &= \frac{\tau}{1!}\left[\frac{\mathrm{d}\mathcal{L}^\varepsilon_{\mathrm{h},\tau}(\xi)}{\mathrm{d}\tau}\bigg|_{r=R^\varepsilon_{\max,\tau}(\xi^0,\theta,\varphi)} + \frac{\partial\mathcal{L}^\varepsilon_{\mathrm{h},\tau}(\xi)}{\partial r}\bigg|_{r=R^\varepsilon_{\max,\tau}(\xi^0,\theta,\varphi)} \frac{\mathrm{d}R^\varepsilon_{\max,\tau}(\xi^0,\theta,\varphi)}{\mathrm{d}\tau}\right]\Bigg|_{\tau=0} + \mathcal{O}(\tau^2) \end{aligned}$$

Solving for the derivative of $R^\varepsilon_{\max,\tau}(\xi^0,\theta,\varphi)$ with respect to τ and inserting the result into the intermediate expression for the second variation of the regularized causal action leads to

$$\begin{aligned} &\big(\delta^2\Sigma_{\mathrm{h}}(\mathrm{P}^\varepsilon_0)\big)(\delta\mathrm{P}^\varepsilon,\delta^2\mathrm{P}^\varepsilon) = \\ &= \frac{1}{2}\int_{\mathbb{R}}\mathrm{d}\xi^0\int_{S^2}\mathrm{d}\Omega_\xi\left[\int_0^{R^\varepsilon_{\max}(\xi^0)}\mathrm{d}r\ r^2\frac{\mathrm{d}^2\mathcal{L}^\varepsilon_{\mathrm{h},\tau}(\xi)}{\mathrm{d}\tau^2}\bigg|_{\tau=0} - \left[\frac{r^2}{\partial_r\mathcal{L}^\varepsilon(\xi)}\left(\frac{\mathrm{d}\mathcal{L}^\varepsilon_{\mathrm{h},\tau}(\xi)}{\mathrm{d}\tau}\bigg|_{\tau=0}\right)^2\right]\Bigg|_{r=R^\varepsilon_{\max}(\xi^0)}\right] \end{aligned}$$

Expressing this result in terms of $\delta\mathcal{L}^\varepsilon_{\mathrm{h}} = \frac{\mathrm{d}\mathcal{L}^\varepsilon}{\mathrm{d}\tau}\big|_{\tau=0}$ and $\delta^2\mathcal{L}^\varepsilon = \frac{1}{2}\frac{\mathrm{d}^2\mathcal{L}^\varepsilon}{\mathrm{d}\tau^2}\big|_{\tau=0}$ and denoting the second variation as $\delta^2\mathcal{S}^\varepsilon_{\mathrm{h}}$ finally yields

$$\delta^2\mathcal{S}^\varepsilon_{\mathrm{h}} = \frac{1}{2}\int_{\mathbb{R}}\mathrm{d}\xi^0\int_{S^2}\mathrm{d}\Omega_\xi\left[\int_0^{R^\varepsilon_{\max}(\xi^0)}\mathrm{d}r\ 2r^2\delta^2\mathcal{L}^\varepsilon(\xi) - \left(r^2\frac{\big(\delta\mathcal{L}^\varepsilon(\xi)\big)^2}{\partial_r\mathcal{L}^\varepsilon(\xi)}\right)\bigg|_{r=R^\varepsilon_{\max}(\xi^0)}\right]$$

In the same way as before, the variations $\delta\mathcal{L}^\varepsilon_{\mathrm{h}}$ and $\delta^2\mathcal{L}^\varepsilon_{\mathrm{h}}$ must be understood as functions of the variations $\delta\mathrm{P}^\varepsilon$ and $\delta^2\mathrm{P}^\varepsilon$ as given in (3.26a) and (3.26b), respectively.

This conclues the proof. □

[a] The point of view that the (unregularized) kernel of the fermionic projector is regarded as a tempered distribution was already mentioned in Footnote 19 on page 33. For a more in-depth discussion we refer to Finster's second book.[11, Lem. 1.2.8]

4

Derivation of the Multipole Expansion of Variations of the Regularized Causal Action

Contents

Having derived an expression for the variation of the regularized causal action in terms of the variation of the regularized causal Lagrangian, we now take this result as our starting point and go one step further: By first decomposing the variations of the regularized kernel of the fermionic projector into Fourier modes and subsequently expanding the latter into scalar and vector spherical harmonics, we can derive multipole expansions

$$\delta\mathcal{S}^\varepsilon = \sum_{l=0}^{\infty} \delta\mathcal{S}_l^\varepsilon\,[\Delta_l^{(1)}] \qquad \text{and} \qquad \delta^2\mathcal{S}^\varepsilon = \sum_{l=0}^{\infty} \delta^2\mathcal{S}_l^\varepsilon\,[\Delta_l^{(1)}, \Delta_l^{(2)}]$$

where the multipole moments $\delta\mathcal{S}_l^\varepsilon$ and $\delta^2\mathcal{S}_l^\varepsilon$ are functionals of the multipole moments $\Delta_{lm}^{(n)}$ (for $-l \leq m \leq l$) of the first ($n = 1$) and second ($n = 2$) variations of the regularized kernel of the fermionic projector in momentum space. The significance of these multipole expansions can best be understood from a comparison with theoretical physics: In much the same way as the details of the angular dependence of electromagnetic and gravitational potentials can be described using spherical harmonics and reflect the shape of the underlying charge and mass distributions, the multipole expansions of the variations of the regularized causal action provide information regarding the question how deviations from a spherically-symmetrically regularized kernel of the fermionic projector affect the regularized causal action. The goal of this chapter is to derive, in a step-by-step approach, expressions for the multipole moments $\delta\mathcal{S}_l^\varepsilon$ and $\delta^2\mathcal{S}_l^\varepsilon$ which will ultimately turn out to be regularization-dependent integral operators with matrix-valued integral kernels. These expressions as given in Theorem 4.3.1 will, in turn, serve as the starting point for further investigations in Part III: Applications.

4.1 Multipole Expansion of the Variations of P^ε and $\mathcal{L}^\varepsilon$

In Subsection 4.1.1 we start by expanding the variation of the regularized kernel of the fermionic projector in momentum space into a multipole series which requires not only ordinary scalar spherical harmonics but also their vectorial counterparts. Subsequently, in Subsection 4.1.2 we decompose the variation of the regularized causal Lagrangian into multipole moments of the Fourier modes of the variation of the regularized kernel of the fermionic projector computed before.

4.1.1 Variation of the Regularized Kernel of the Fermionic Projector

In the following sections and chapters we always consider regularized kernels $\widehat{\mathrm{P}^\varepsilon_\tau} \in \mathcal{D}'(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4, \mathbb{C}^4))$ of the fermionic projector in momentum space which must be understood as the Fourier modes of a regularized kernel of the fermionic projector as discussed in Section 3.2. The subscript τ indicates that $\widehat{\mathrm{P}^\varepsilon_\tau}$ is obtained from the minimizer $\widehat{\mathrm{P}^\varepsilon_0}$ by "slightly" deforming the regularization such that $\widehat{\mathrm{P}^\varepsilon_\tau}$ does in general no longer minimize the regularized causal action.

Definition 4.1.1 (Perturbed Regularized Kernel of the Fermionic Projector)

In momentum space, the *perturbed regularized kernel of the fermionic projector* takes the form

$$\widehat{\mathrm{P}^\varepsilon_\tau}(p) = \sum_{i=0}^{3} \widehat{v^\varepsilon_{\tau,i}}(p)\gamma^i + \widehat{s^\varepsilon}(p)\mathrm{id}_{\mathbb{C}^4} \tag{4.1}$$

where $\gamma^0, \ldots, \gamma^3$ denote the Dirac gamma matrices and where the vector and scalar component distributions are given in terms of the functions $a_\tau, b^\alpha_\tau, c_\tau \in \mathcal{D}'(\mathbb{R}^4, \mathbb{R})$ as follows

$$\widehat{v^\varepsilon_{\tau,0}}(p) := a_\tau(p)\delta\big(\sigma^\varepsilon_\tau(p)\big)\Theta(-p^0) \tag{4.1a}$$

$$\widehat{v^\varepsilon_{\tau,\alpha}}(p) := -b^\alpha_\tau(p)\delta\big(\sigma^\varepsilon_\tau(p)\big)\Theta(-p^0) \tag{4.1b}$$

$$\widehat{s^\varepsilon_\tau}(p) := c_\tau(p)\delta\big(\sigma^\varepsilon_\tau(p)\big)\Theta(-p^0) \tag{4.1c}$$

Here the argument of the Dirac δ-distributions is the *deformed regularized mass shell* given by

$$\sigma^\varepsilon_\tau(p) = p^2 - \mu^\varepsilon_\tau(p) \qquad \text{with} \qquad \sigma^\varepsilon_0(p) = p^2 - \mu^\varepsilon_0(p) \tag{4.2}$$

where the functions $\mu^\varepsilon_\tau \in C^\infty(\mathbb{R}^4, \mathbb{R})$ are deformed versions of the regularized mass shell $\mu^\varepsilon_0 \in C^\infty(\mathbb{R}^4, \mathbb{R})$ which reduces to $\mu^0_0(p) = \mu^2$ for vanishing regularization.[a]

[a] Note that the mass shell parameter will be denoted by μ rather than m in order to avoid confusion with the multipole parameter m.

Starting from this expression, one can now calculate the variation of the regularized kernel of the fermionic projector around the minimizer $\widehat{\mathrm{P}^\varepsilon_0}$ which, according to the above ansatz, does in principle yield two contributions: On the one hand, there are variations which are due to changes in the coefficient functions a_0, b^α_0, c_0 while, on the other hand, one also obtains variations originating from a deformation of the mass shell $\mu^\varepsilon_0 \in C^\infty(\mathbb{R}^4, \mathbb{R})$. In the most general case, of course, both contributions have to be taken into account – for reasons of manageability, however, we restrict our considerations as follows.

Assumption 4.1.2 (Variation of $\widehat{\mathrm{P}^\varepsilon_0}$ and Rank Condition)

In what follows, variations of the regularized kernel of the fermionic projector always mean variations of the component functions $a_0, b^\alpha_0, c_0 \in \mathcal{D}'(\mathbb{R}^4, \mathbb{R})$ while variations of the regularized mass shell will be disregarded. Thus, the variation of the components of the regularized kernel of the fermionic projector for $n = 1, 2$ always take the form

$$\widehat{\delta^{(n)} v_0^\varepsilon}(p) = \delta^{(n)} a(p) \delta\big(\sigma^\varepsilon(p)\big) \Theta(-p^0) \tag{4.3a}$$

$$\widehat{\delta^{(n)} v_\alpha^\varepsilon}(p) = -\delta^{(n)} b^\alpha(p) \delta\big(\sigma^\varepsilon(p)\big) \Theta(-p^0) \tag{4.3b}$$

$$\widehat{\delta^{(n)} s^\varepsilon}(p) = \delta^{(n)} c(p) \delta\big(\sigma^\varepsilon(p)\big) \Theta(-p^0) \tag{4.3c}$$

where $\sigma^\varepsilon \equiv \sigma_0^\varepsilon(p) = p^2 - \mu_0^\varepsilon(p)$ denotes the undeformed regularized mass shell.

In addition to this, only deformations for which $\widehat{\mathrm{P}_\tau^\varepsilon}$ still has rank two and projects onto the subspace of negative-energy solutions of the Dirac equation are admissible.

Optimizing the Regularization
As already explained in Section 1.3, it is the causal action principle that introduces dynamics within the theory of causal fermion systems. When applied to a concrete physical situation where spacetime and its matter content is modelled through a regularized kernel of the fermionic projector, the causal action principle is aimed at adjusting the regularization encoded in the regularized kernel of the fermionic projector in such a way that the causal action is minimized. The resulting regularization corresponds to an optimal microstructure of physical spacetime. In what follows, we will replace a spherically-symmetrically regularized kernel of the fermionic projector by an anisotropically regularized one and study the consequences on $\mathcal{S}^\varepsilon$.

Scalar and Vector Spherical Harmonics Expansion
In order to allow for a systematic analysis of the effect of anisotropic deformations of the regularization on $\mathcal{S}^\varepsilon$, we have to work out the dependence of the variations $\delta\mathcal{S}^\varepsilon$ and $\delta^2\mathcal{S}^\varepsilon$ on the multipole moments of the momentum space variations $\delta\widehat{\mathrm{P}^\varepsilon}$ and $\delta^2\widehat{\mathrm{P}^\varepsilon}$. To this end, we not only need the ordinary scalar spherical harmonics, but also their vectorial analogues.

Definition 4.1.3 (Vector Spherical Harmonics)

For $(l, m) \in \mathbb{N}_0 \times \mathbb{Z}$ with $-l \leq m \leq l$, the *vector spherical harmonics* $\vec{Y}_{lm}, \vec{\Psi}_{lm}, \vec{\Phi}_{lm} : S^2 \to \mathbb{C}^3$ are the functions defined as[74]

$$(\theta, \varphi) \mapsto \vec{Y}_{lm}(\theta, \varphi) := Y_{lm}(\theta, \varphi) \frac{\vec{r}}{|\vec{r}|} \tag{4.4a}$$

$$(\theta, \varphi) \mapsto \vec{\Psi}_{lm}(\theta, \varphi) := |\vec{r}| (\operatorname{grad} Y_{lm})(\theta, \varphi) \tag{4.4b}$$

$$(\theta, \varphi) \mapsto \vec{\Phi}_{lm}(\theta, \varphi) := \vec{r} \times (\operatorname{grad} Y_{lm})(\theta, \varphi) \tag{4.4c}$$

where $Y_{lm} : S^2 \to \mathbb{C}$ are the ordinary (scalar) spherical harmonics which, in terms of the associated Legendre polynomials $P_{lm} : [-1, 1] \to \mathbb{R}$, are explicitly given by[a]

$$(\theta, \varphi) \mapsto Y_{lm}(\theta, \varphi) := (-1)^m \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-m)!}{(l+m)!}} P_{lm}(\cos(\theta)) \mathrm{e}^{im\varphi} \tag{4.5a}$$

with

$$x \mapsto P_{lm}(x) := (1 - x^2)^{\frac{m}{2}} \frac{\mathrm{d}^m P_l}{\mathrm{d}x^m}(x) \qquad \text{and} \qquad x \mapsto P_l(x) := \frac{1}{2^l l!} \frac{\mathrm{d}^l}{\mathrm{d}x^l}(x^2 - 1)^l \tag{4.5b}$$

[a]Note that there exist different conventions concerning the prefactors of the spherical harmonics. Here we follow the convention used in standard textbooks on quantum mechanics such as the one by Messiah[75, eq. (B. 93)]. We remark that this convention also coincides with the one used in the standard textbook on classical electrodynamics by Jackson[76, eq. (3.53)], with the slight difference that in the latter the phase factor $(-1)^m$ is absorbed in the definition of the associated Legendre polynomials.

Making use of the ordinary spherical harmonics as well as their vectorial analogues, the vector and scalar components of the variations of the regularized kernel of the fermionic projector as given in Assumption 4.1.2 can be decomposed into multipole moments as follows

$$\delta^{(n)}a(p) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \delta^{(n)}a_{lm}(p^0,|\vec{p}|)Y_{lm} \tag{4.6a}$$

$$\delta^{(n)}b^\alpha(p) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \Big[\delta^{(n)}b^{(1)}_{lm}(p^0,|\vec{p}|)Y^\alpha_{lm} + \delta^{(n)}b^{(2)}_{lm}(p^0,|\vec{p}|)\Psi^\alpha_{lm} + \delta^{(n)}b^{(3)}_{lm}(p^0,|\vec{p}|)\Phi^\alpha_{lm}\Big] \tag{4.6b}$$

$$\delta^{(n)}c(p) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \delta^{(n)}c_{lm}(p^0,|\vec{p}|)Y_{lm} \tag{4.6c}$$

where we have suppressed the arguments of the scalar and vector spherical harmonics.[1] For the vector variation $\delta^{(n)}b^\alpha$ we implicitly defined $Y^\alpha_{lm} := \vec{Y}_{lm}\cdot\vec{e}_\alpha$, $\Psi^\alpha_{lm} := \vec{\Psi}_{lm}\cdot\vec{e}_\alpha$, $\Phi^\alpha_{lm} := \vec{\Phi}_{lm}\cdot\vec{e}_\alpha$ as the scalar products of the vector spherical harmonics with the α^{th} Cartesian unit vector in $\mathbb{R}^3$. For notational convenience we furthermore combine the multipole moments $\delta^{(n)}a_{lm}$, $\delta^{(n)}b^{(1,2,3)}_{lm}$ and $\delta^{(n)}c_{lm}$ into five-component, complex-valued vectors.

Definition 4.1.4 (Vector of Multipole Moments of Variations)

For $n \in \{1,2\}$ and $(l,m) \in \mathbb{N}_0 \times \mathbb{Z}$ with $-l \le m \le l$, the functions $(\Delta^{(n)})_{lm} \in \mathcal{D}'(\mathbb{R}\times\mathbb{R}^+_0,\mathbb{C}^5)$, referred to as the *vectors of multipole moments at order* n, are defined as

$$\Delta^{(1)}_{lm}(p^0,|\vec{p}|) = \begin{pmatrix}\delta a_{lm}(p^0,|\vec{p}|)\\ \delta b^{(1)}_{lm}(p^0,|\vec{p}|)\\ \delta b^{(2)}_{lm}(p^0,|\vec{p}|)\\ \delta b^{(3)}_{lm}(p^0,|\vec{p}|)\\ \delta c_{lm}(p^0,|\vec{p}|)\end{pmatrix} \tag{4.7a}$$

$$(\Delta^{(2)})_{lm}(p^0,|\vec{p}|) = \begin{pmatrix}\delta^2 a_{lm}(p^0,|\vec{p}|)\\ \delta^2 b^{(1)}_{lm}(p^0,|\vec{p}|)\\ \delta^2 b^{(2)}_{lm}(p^0,|\vec{p}|)\\ \delta^2 b^{(3)}_{lm}(p^0,|\vec{p}|)\\ \delta^2 c_{lm}(p^0,|\vec{p}|)\end{pmatrix} \tag{4.7b}$$

4.1.2 Variation of the Regularized Causal Lagrangian

Having expanded the variation of the regularized kernel of the fermionic projector into a multipole series, we next decompose the variation of the regularized causal Lagrangian from Lemma 3.4.2 into Fourier modes and subsequently express everything in terms of the multipole moments $\Delta^{(1)}_{lm}$ and $(\Delta^{(2)})_{lm}$. Before, however, we introduce some abbreviating notation and terminology for frequently occurring expressions.

Definition 4.1.5 (Hadamard Product)

For any two matrices $A, B \in \mathbb{C}^{m\times n}$ their *Hadamard product* $A \odot B$ is defined as the entrywise product

$$(A\odot B)_{ij} = A_{ij}B_{ij} \tag{4.8}$$

[1] We will employ this practice of simplification of notation whenever there is no risk of confusion. Furthermore, we will abbreviate sums over multipole indices as $\sum_{l,m}$ without specifying $(l,m) \in \mathbb{N}_0\times\mathbb{Z}$ where $-l \le m \le l$.

Definition 4.1.6 (Matrices of Spherical Harmonics)

The *matrices of spherical harmonics* are defined as

$$\Upsilon_{lm} := \operatorname{diag}\Big(Y_{lm}, \xi^\alpha Y^\alpha_{lm}, \xi^\alpha \Psi^\alpha_{lm}, \xi^\alpha \Phi^\alpha_{lm}, Y_{lm}\Big) \tag{4.9a}$$

$$\Upsilon_{lm|l'm'} := \begin{pmatrix} Y_{lm}Y_{l'm'} & Y_{lm}\xi^\beta \begin{bmatrix} Y^\beta_{l'm'} & \Psi^\beta_{l'm'} & \Phi^\beta_{l'm'} \end{bmatrix} & Y_{lm}Y_{l'm'} \\ \xi^\alpha \begin{bmatrix} Y^\alpha_{lm} \\ \Psi^\alpha_{lm} \\ \Phi^\alpha_{lm} \end{bmatrix} Y_{l'm'} & \xi^\alpha\xi^\beta \begin{bmatrix} Y^\alpha_{lm}Y^\beta_{l'm'} & Y^\alpha_{lm}\Psi^\beta_{l'm'} & Y^\alpha_{lm}\Phi^\beta_{l'm'} \\ \Psi^\alpha_{lm}Y^\beta_{l'm'} & \Psi^\alpha_{lm}\Psi^\beta_{l'm'} & \Psi^\alpha_{lm}\Phi^\beta_{l'm'} \\ \Phi^\alpha_{lm}Y^\beta_{l'm'} & \Phi^\alpha_{lm}\Psi^\beta_{l'm'} & \Phi^\alpha_{lm}\Phi^\beta_{l'm'} \end{bmatrix} & \xi^\alpha \begin{bmatrix} Y^\alpha_{lm} \\ \Psi^\alpha_{lm} \\ \Phi^\alpha_{lm} \end{bmatrix} Y_{l'm'} \\ Y_{lm}Y_{l'm'} & Y_{lm}\xi^\beta \begin{bmatrix} Y^\beta_{l'm'} & \Psi^\beta_{l'm'} & \Phi^\beta_{l'm'} \end{bmatrix} & Y_{lm}Y_{l'm'} \end{pmatrix} \tag{4.9b}$$

$$\overset{*}{\Upsilon}_{lm|l'm'} := \begin{pmatrix} 0 & \begin{bmatrix} 0 & 0 & 0 \end{bmatrix} & 0 \\ \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} & \begin{bmatrix} Y^\alpha_{lm}Y^\alpha_{l'm'} & Y^\alpha_{lm}\Psi^\alpha_{l'm'} & Y^\alpha_{lm}\Phi^\alpha_{l'm'} \\ \Psi^\alpha_{lm}Y^\alpha_{l'm'} & \Psi^\alpha_{lm}\Psi^\alpha_{l'm'} & \Psi^\alpha_{lm}\Phi^\alpha_{l'm'} \\ \Phi^\alpha_{lm}Y^\alpha_{l'm'} & \Phi^\alpha_{lm}\Psi^\alpha_{l'm'} & \Phi^\alpha_{lm}\Phi^\alpha_{l'm'} \end{bmatrix} & \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \\ 0 & \begin{bmatrix} 0 & 0 & 0 \end{bmatrix} & 0 \end{pmatrix} \tag{4.9c}$$

where ξ^α is the α^{th} component of $\vec{\xi} \in \mathbb{R}^3$ with respect to the standard basis. Furthermore, doubly occurring Greek indices are understood as triggering a summation from 1 to 3.

The apparent internal block matrix structure of these matrices of spherical harmonics will become relevant later on, especially for the explicit computations in Appendix C. For the sake of completeness, we therefore introduce the following terminology for the different blocks of the matrix.

Terminology 4.1.7 (Dotted, Double-Dotted and Asterisked Terms)

For the different blocks of the matrices $\Upsilon_{lm|l'm'}$ and $\overset{*}{\Upsilon}_{lm|l'm'}$ we introduce the following terminology, which is chosen with mnemonic aspects[a] in mind:

- *Dotted Terms*
  - *Dotted-unprimed terms* are those parts of the matrices which are proportional to the (3×1) block matrix $(Y^\alpha_{lm}, \Psi^\alpha_{lm}, \Phi^\alpha_{lm})^{\mathrm{T}}$
  - *Dotted-primed terms* are those parts of the matrices which are proportional to the (1×3) block matrix $(Y^\beta_{l'm'}, \Psi^\beta_{l'm'}, \Phi^\beta_{l'm'})$
- *Double-dotted terms* are those parts of the matrices which are proportional to the (3×3) block matrix with entries $\mathbf{Y}^\alpha_{lm}\mathbf{Y}^\beta_{l'm'}$ where $\vec{\mathbf{Y}}_{l^{(\prime)}m^{(\prime)}} \in \{\vec{Y}_{l^{(\prime)}m^{(\prime)}}, \vec{\Phi}_{l^{(\prime)}m^{(\prime)}}, \vec{\Psi}_{l^{(\prime)}m^{(\prime)}}\}$
- *Asterisked terms* are those parts of the matrices which are proportional to the (3×3) block matrix with entries $\mathbf{Y}^\alpha_{lm}\mathbf{Y}^\alpha_{l'm'}$ where $\vec{\mathbf{Y}}_{l^{(\prime)}m^{(\prime)}} \in \{\vec{Y}_{l^{(\prime)}m^{(\prime)}}, \vec{\Phi}_{l^{(\prime)}m^{(\prime)}}, \vec{\Psi}_{l^{(\prime)}m^{(\prime)}}\}$

[a] The underlying idea of this terminology is the following: Dotted and double-dotted terms all originate from scalar products of vector spherical harmonics $\vec{\mathbf{Y}}_{l^{(\prime)}m^{(\prime)}}$ with $\vec{\xi}$. The number of dots indicates the number of scalar products involved, i. e. one scalar product in $\vec{\xi} \cdot \vec{\mathbf{Y}}_{lm}$ (dotted-*unprimed* terms) and $\vec{\xi} \cdot \vec{\mathbf{Y}}_{l'm'}$ (dotted-*primed* terms), but two scalar products in $(\vec{\xi} \cdot \vec{\mathbf{Y}}_{lm})(\vec{\xi} \cdot \vec{\mathbf{Y}}_{l'm'})$. In contrast, the asterisk indicates that vector spherical harmonics $\vec{\mathbf{Y}}_{l^{(\prime)}m^{(\prime)}}$ form scalar products with themselves.

Making use of these matrices of spherical harmonics, the variation of the regularized causal Lagrangian can be expanded in a multipole series.

Lemma 4.1.8 (Multipole Expansion of $\delta\mathcal{L}^\varepsilon$)

Let the spatial part of the vector component functions v^ε_α of the *unperturbed* regularized kernel of the fermionic projector take the form

$$v^\varepsilon_\alpha(\xi) = -\xi^\alpha v^\varepsilon(\xi) \tag{4.10}$$

with $v^\varepsilon \in \mathcal{D}'(\mathbb{R}^4, \mathbb{C})$. Then the multipole expansion and Fourier decomposition of the first variation $\delta\mathcal{L}^\varepsilon(\xi)$ of the regularized causal Lagrangian as derived in Lemma 3.4.2 takes the form

$$\delta\mathcal{L}^\varepsilon(\xi) = \sum_{l,m} \mathrm{Re}\left\{ \int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}}{(2\pi)^4}\; \mathbb{1}_{1\times 5}\, \mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})\Delta^\varepsilon_{lm}(|\vec{p}|) \right\} \tag{4.11}$$

where the matrix-valued functions $\mathcal{K}^\varepsilon_{lm}$ for all $(l,m) \in \mathbb{N}_0 \times \mathbb{Z}$ with $-l \le m \le l$ are defined in terms of a Hadamard product as

$$\mathcal{K}^\varepsilon_{lm}(\xi,\vec{p}) \overset{(4.9a)}{=} \left[\mathcal{C}^\varepsilon_{\mathcal{K}} \odot \Upsilon_{lm}\right] E^\varepsilon_{\mathcal{K}} \mathrm{e}^{-\mathrm{i}\vec{p}\cdot\vec{\xi}} \tag{4.11a}$$

with the *coefficient matrix* $\mathcal{C}^\varepsilon_{\mathcal{K}} : \mathbb{R}^4 \to \mathbb{C}^{5\times 5}$ and the function $E^\varepsilon_{\mathcal{K}} : \mathbb{R} \times \mathbb{R}^+_0 \to \mathbb{C}$ as given in (4.13a) and (4.13b), respectively.

Proof. Decomposing the perturbations $\delta v^\varepsilon_i(\xi)$ and $\delta s^\varepsilon(\xi)$ into Fourier modes according to

$$\delta v^\varepsilon_i(\xi) = \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\; \widehat{\delta v^\varepsilon_i}(p)\mathrm{e}^{\mathrm{i}p\xi} \tag{4.12a}$$

$$\delta s^\varepsilon(\xi) = \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\; \widehat{\delta s^\varepsilon}(p)\mathrm{e}^{\mathrm{i}p\xi} \tag{4.12b}$$

and replacing all occurrences of $\delta v^\varepsilon_i(\xi)$ and $\delta s^\varepsilon(\xi)$ in (3.26a) by these expressions, we find

$$\delta\mathcal{L}^\varepsilon(\xi) \overset{(3.26a)}{\underset{(4.12)}{=}} 16\,\mathrm{Re}\left\{ \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4} \left[\eta^{ij}\big(B^\varepsilon\overline{v^\varepsilon_i} - C^\varepsilon v^\varepsilon_i\big)\widehat{\delta v^\varepsilon_j}(p) + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\widehat{\delta s^\varepsilon}(p)\right]\mathrm{e}^{\mathrm{i}p\xi} \right\}$$

where we suppress the position space argument ξ both in the functions B^ε, C^ε and in the vector and scalar components v^ε_i, s^ε. Next, we insert the variations of the vector and scalar component from (4.3) along with their multipole expansion as given in (4.6) and thus arrive at

$$\begin{aligned}\delta\mathcal{L}^\varepsilon(\xi) \overset{(4.3)}{\underset{(4.6)}{=}} 16\sum_{l,m}\mathrm{Re}\Bigg\{ \int_{\mathbb{R}} \mathrm{d}p^0 \int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}}{(2\pi)^4} &\left[\frac{\delta\big(p^0+\omega^\varepsilon_p\big)\Theta(-p^0)\mathrm{e}^{\mathrm{i}p\xi}}{|\partial_{p^0}\sigma^\varepsilon(p^0,|\vec{p}|)|_{p^0=-\omega^\varepsilon_p}|} + \frac{\delta\big(p^0-\omega^\varepsilon_p\big)\Theta(-p^0)\mathrm{e}^{\mathrm{i}p\xi}}{|\partial_{p^0}\sigma^\varepsilon(p^0,|\vec{p}|)|_{p^0=+\omega^\varepsilon_p}|}\right]\times \\ &\times\Bigg[\big(B^\varepsilon\overline{v^\varepsilon_0} - C^\varepsilon v^\varepsilon_0\big)\delta a_{lm}(p^0,|\vec{p}|)Y_{lm} + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta c_{lm}(p^0,|\vec{p}|)Y_{lm} \\ &- \big(B^\varepsilon\overline{v^\varepsilon_\alpha} - C^\varepsilon v^\varepsilon_\alpha\big)\Big(\delta b^{(1)}_{lm}(p^0,|\vec{p}|)Y^\alpha_{lm} + \delta b^{(2)}_{lm}(p^0,|\vec{p}|)\Psi^\alpha_{lm} + \delta b^{(3)}_{lm}(p^0,|\vec{p}|)\Phi^\alpha_{lm}\Big)\Bigg]\Bigg\}\end{aligned}$$

where we have rewritten the composition of the δ-distribution with the regularized mass shell σ^ε in terms of the zeroes $p^0 = \pm\omega^\varepsilon_p$ of $\sigma^\varepsilon(p^0,|\vec{p}|)$. Carrying out the p^0-integral and expressing the integrand in terms of the vector Δ_{lm} of multipole moments and the matrix of spherical harmonics Υ_{lm} as introduced in (4.7) and (4.9a), respectively, we end up with

$$\delta\mathcal{L}^\varepsilon(\xi) \overset{(4.7)}{\underset{(4.9a)}{=}} \sum_{l,m}\mathrm{Re}\left\{ \int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}}{(2\pi)^4}\; \mathbb{1}_{1\times 5}\left[\big(\mathcal{C}^\varepsilon_{\mathcal{K}} \odot \Upsilon_{lm}\big)E^\varepsilon_{\mathcal{K}}\mathrm{e}^{-\mathrm{i}\vec{p}\cdot\vec{\xi}}\right]\Delta_{lm}\big(-\omega^\varepsilon_p,|\vec{p}|\big) \right\} \tag{4.13}$$

where the *coefficient matrix* $\mathcal{C}^\varepsilon_{\mathcal{K}} : \mathbb{R}^4 \to \mathbb{C}^{5\times 5}$ and the function $E^\varepsilon_{\mathcal{K}} : \mathbb{R} \times \mathbb{R}^+_0 \to \mathbb{C}$ are defined as

$$\mathcal{C}^\varepsilon_{\mathcal{K}}(\xi) = \operatorname{diag}\Big(\big(B^\varepsilon \overline{v^\varepsilon_0} - C^\varepsilon v^\varepsilon_0\big) \ , \ -\big(B^\varepsilon \overline{v^\varepsilon} - C^\varepsilon v^\varepsilon\big)\mathrm{id}_{\mathbb{C}^3} \ , \ \big(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\Big) \tag{4.13a}$$

$$E^\varepsilon_{\mathcal{K}}(\xi^0, |\vec{p}|) = \frac{16\mathrm{e}^{\mathrm{i}p^0\xi^0}}{\big|\partial_{p^0}\sigma^\varepsilon(p^0,|\vec{p}|)\big|}\Bigg|_{p^0=-\omega^\varepsilon_p} \tag{4.13b}$$

respectively. Taken together, the expression in square brackets in (4.13) will be denoted by

$$\mathcal{K}^\varepsilon_{lm}(\xi,\vec{p}) := \big(\mathcal{C}^\varepsilon_{\mathcal{K}} \odot \Upsilon_{lm}\big) E^\varepsilon_{\mathcal{K}} \mathrm{e}^{-\mathrm{i}\vec{p}\cdot\vec{\xi}} \tag{4.14}$$

where we usually suppress all the arguments. As a consequence of the regularization of the mass shell, the multipole moments Δ_{lm} acquire a dependence on the regularization through ω^ε_p. We define

$$(\Delta^{(n)})^\varepsilon_{lm}(|\vec{p}|) := (\Delta^{(n)})_{lm}(-\omega^\varepsilon_p, |\vec{p}|) \tag{4.15}$$

for every $n \in \mathbb{N}$. This concludes the proof. □

In the same way as for the first variation of the regularized causal Lagrangian, we also expand the second variation into a multipole series, where now the matrices $\Upsilon_{lm|l'm'}$ and $\overset{*}{\Upsilon}_{lm|l'm'}$ appear.

Lemma 4.1.9 (Multipole Expansion of $\delta^2\mathcal{L}^\varepsilon$)

Let the spatial part of the vector component functions v^ε_α of the *unperturbed* regularized kernel of the fermionic projector again take the form

$$v^\varepsilon_\alpha(\xi) = -\xi^\alpha v^\varepsilon(\xi) \tag{4.16}$$

with $v^\varepsilon \in \mathcal{D}'(\mathbb{R}^4, \mathbb{C})$. Then the multipole expansion and Fourier decomposition of the second variation $\delta^2\mathcal{L}^\varepsilon(\xi)$ of the regularized causal Lagrangian as derived in Lemma 3.4.2 takes the form

$$\begin{aligned}\delta^2\mathcal{L}^\varepsilon(\xi) \overset{(4.7)}{\underset{(4.9b)}{=}} &\sum_{l,m} \mathrm{Re}\left\{\int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}}{(2\pi)^4}\ \mathbb{1}_{1\times 5}\, \mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})(\Delta^2)^\varepsilon_{lm}(|\vec{p}|)\right\}\\ &+\frac{1}{2}\sum_{\substack{l,m\\ l',m'}} \mathrm{Re}\left\{\int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}}{(2\pi)^4}\int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{q}}{(2\pi)^4}\ \Delta^\varepsilon_{lm}(|\vec{p}|)^{\mathrm{T}}\mathcal{M}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q})\Delta^\varepsilon_{l'm'}(|\vec{q}|)\right\}\\ &+\frac{1}{2}\sum_{\substack{l,m\\ l',m'}} \mathrm{Re}\left\{\int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}}{(2\pi)^4}\int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{q}}{(2\pi)^4}\ \Delta^\varepsilon_{lm}(|\vec{p}|)^{\mathrm{T}}\mathcal{N}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q})\overline{\Delta^\varepsilon_{l'(-m')}(|\vec{q}|)}\right\}\end{aligned} \tag{4.17}$$

where the matrix-valued functions $\mathcal{M}^\varepsilon_{lm|l'm'}, \mathcal{N}^\varepsilon_{lm|l'm'}$ for all $(l,m),(l',m') \in \mathbb{N}_0 \times \mathbb{Z}$ with $-m^{(\prime)} \le l^{(\prime)} \le m^{(\prime)}$ are defined in terms of Hadamard products as

$$\mathcal{M}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q}) = \big[\mathcal{C}^\varepsilon_{\mathcal{M}} \odot \Upsilon_{lm|l'm'} + C^\varepsilon \overset{*}{\Upsilon}_{lm|l'm'}\big] E^\varepsilon_{\mathcal{M}} \mathrm{e}^{-\mathrm{i}(\vec{p}+\vec{q})\cdot\vec{\xi}} \tag{4.17a}$$

$$\mathcal{N}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q}) = \big[\mathcal{C}^\varepsilon_{\mathcal{N}} \odot \Upsilon_{lm|l'm'} - B^\varepsilon \overset{*}{\Upsilon}_{lm|l'm'}\big] E^\varepsilon_{\mathcal{N}} \mathrm{e}^{-\mathrm{i}(\vec{p}-\vec{q})\cdot\vec{\xi}} \tag{4.17b}$$

with the coefficient matrices $\mathcal{C}^\varepsilon_{\mathcal{M}}, \mathcal{C}^\varepsilon_{\mathcal{N}} : \mathbb{R}^4 \to \mathbb{C}^{5\times 5}$ and the functions $E^\varepsilon_{\mathcal{M}}, E^\varepsilon_{\mathcal{N}} : \mathbb{R} \times (\mathbb{R}^+_0)^2 \to \mathbb{C}$ as given in (4.19a,i), (4.19b,i) and (4.19a,ii), (4.19b,ii), respectively.

Proof. Decomposing the perturbations $\delta v_i^\varepsilon(\xi)$ and $\delta s^\varepsilon(\xi)$ into Fourier modes according to

$$\delta^{(n)} v_i^\varepsilon(\xi) = \int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\ \widehat{\delta^{(n)} v_i^\varepsilon}(p)\mathrm{e}^{\mathrm{i}p\xi} \qquad (4.18\mathrm{a}) \qquad \delta^{(n)} s^\varepsilon(x,y) = \int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\ \widehat{\delta^{(n)} s^\varepsilon}(p)\mathrm{e}^{\mathrm{i}p\xi} \qquad (4.18\mathrm{b})$$

and replacing all occurrences in (3.26b) by these expressions, we find

$$\begin{aligned}
\delta^2\mathcal{L}^\varepsilon(\xi) \overset{(3.26\mathrm{b})}{=} 16\,\mathrm{Re}\Bigg\{ & \int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\ \Big[\eta^{ij}\big(B^\varepsilon\overline{v_i^\varepsilon} - C^\varepsilon v_i^\varepsilon\big)\widehat{\delta^2 v_j^\varepsilon}(p) + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\widehat{\delta^2 s^\varepsilon}(p)\Big]\mathrm{e}^{\mathrm{i}p\xi} \\
& + \frac{1}{2}\int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 q}{(2\pi)^4}\ \bigg[\Big(\eta^{ij}\eta^{kl}\overline{v_i^\varepsilon v_k^\varepsilon}\widehat{\delta v_j^\varepsilon}(p)\widehat{\delta v_l^\varepsilon}(q) - \eta^{ij}C^\varepsilon\widehat{\delta v_i^\varepsilon}(p)\widehat{\delta v_j^\varepsilon}(q) \\
& \qquad + \eta^{ij}\overline{v_i^\varepsilon}\,\overline{s^\varepsilon}\widehat{\delta v_j^\varepsilon}(p)\widehat{\delta s^\varepsilon}(q) + \eta^{ij}\overline{v_i^\varepsilon}\,\overline{s^\varepsilon}\widehat{\delta s^\varepsilon}(p)\widehat{\delta v_j^\varepsilon}(q) \\
& \qquad + (\overline{v^\varepsilon})^2\widehat{\delta s^\varepsilon}(p)\widehat{\delta s^\varepsilon}(q)\Big) \\
& + \Big(\eta^{ij}\eta^{kl}\big(\overline{v_i^\varepsilon}v_k^\varepsilon - 2v_i^\varepsilon\overline{v_k^\varepsilon}\big)\widehat{\delta v_j^\varepsilon}(p)\widehat{\overline{\delta v_l^\varepsilon}}(q) + \eta^{ij}B^\varepsilon\widehat{\delta v_i^\varepsilon}(p)\widehat{\overline{\delta v_j^\varepsilon}}(q) \\
& \qquad + \eta^{ij}v_i^\varepsilon\overline{s^\varepsilon}\big(\widehat{\delta s^\varepsilon}(p)\widehat{\overline{\delta v_j^\varepsilon}}(q) + 2\widehat{\delta v_j^\varepsilon}(p)\widehat{\overline{\delta s^\varepsilon}}(q)\big) \\
& \qquad + \eta^{ij}v_i^\varepsilon\overline{s^\varepsilon}\big(\widehat{\delta s^\varepsilon}(q)\widehat{\overline{\delta v_j^\varepsilon}}(p) + 2\widehat{\delta v_j^\varepsilon}(q)\widehat{\overline{\delta s^\varepsilon}}(p)\big) + |v^\varepsilon|^2\widehat{\delta s^\varepsilon}(p)\widehat{\overline{\delta s^\varepsilon}}(q)\Big)\bigg]\mathrm{e}^{\mathrm{i}(p+q)\xi}\Bigg\}
\end{aligned}$$

where we symmetrized the terms containing first-order variations of both the vector and scalar component with regard to complex conjugations by exploiting the presence of the real part. Making use of the fact that variations and complex conjugations commute, which in momentum space amounts to

$$\widehat{\overline{\delta v_i^\varepsilon}}(p)\mathrm{e}^{\mathrm{i}p\xi} = \overline{\widehat{\delta v_i^\varepsilon}}(p)\mathrm{e}^{-\mathrm{i}p\xi}$$

the second variation of the regularized causal Lagrangian turns into the form

$$\begin{aligned}
\delta^2\mathcal{L}^\varepsilon(\xi) = 16\,\mathrm{Re}\Bigg\{ & \int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\ \Big[\eta^{ij}\big(B^\varepsilon\overline{v_i^\varepsilon} - C^\varepsilon v_i^\varepsilon\big)\widehat{\delta^2 v_j^\varepsilon}(p) + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\widehat{\delta^2 s^\varepsilon}(p)\Big]\mathrm{e}^{\mathrm{i}p\xi} \\
& + \frac{1}{2}\int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 q}{(2\pi)^4}\ \bigg[\Big(\eta^{ij}\eta^{kl}\overline{v_i^\varepsilon v_k^\varepsilon}\widehat{\delta v_j^\varepsilon}(p)\widehat{\delta v_l^\varepsilon}(q) - \eta^{ij}C^\varepsilon\widehat{\delta v_i^\varepsilon}(p)\widehat{\delta v_j^\varepsilon}(q) \\
& \qquad + \eta^{ij}\overline{v_i^\varepsilon}\,\overline{s^\varepsilon}\widehat{\delta v_j^\varepsilon}(p)\widehat{\delta s^\varepsilon}(q) + \eta^{ij}\overline{v_i^\varepsilon}\,\overline{s^\varepsilon}\widehat{\delta s^\varepsilon}(p)\widehat{\delta v_j^\varepsilon}(q) \\
& \qquad + (\overline{v^\varepsilon})^2\widehat{\delta s^\varepsilon}(p)\widehat{\delta s^\varepsilon}(q)\Big)\mathrm{e}^{\mathrm{i}(p+q)\xi} \\
& + \Big(\eta^{ij}\eta^{kl}\big(\overline{v_i^\varepsilon}v_k^\varepsilon - 2v_i^\varepsilon\overline{v_k^\varepsilon}\big)\widehat{\delta v_j^\varepsilon}(p)\overline{\widehat{\delta v_l^\varepsilon}}(q) + \eta^{ij}B^\varepsilon\widehat{\delta v_i^\varepsilon}(p)\overline{\widehat{\delta v_j^\varepsilon}}(q) \\
& \qquad + \eta^{ij}v_i^\varepsilon\overline{s^\varepsilon}\big(\widehat{\delta s^\varepsilon}(p)\overline{\widehat{\delta v_j^\varepsilon}}(q) + 2\widehat{\delta v_j^\varepsilon}(p)\overline{\widehat{\delta s^\varepsilon}}(q)\big) \\
& \qquad + \eta^{ij}\overline{v_i^\varepsilon}s^\varepsilon\big(\widehat{\delta v_j^\varepsilon}(p)\overline{\widehat{\delta s^\varepsilon}}(q) + 2\widehat{\delta s^\varepsilon}(p)\overline{\widehat{\delta v_j^\varepsilon}}(q)\big) + |v^\varepsilon|^2\widehat{\delta s^\varepsilon}(p)\overline{\widehat{\delta s^\varepsilon}}(q)\Big)\mathrm{e}^{\mathrm{i}(p-q)\xi}\bigg]\Bigg\}
\end{aligned}$$

where we once more exploited the presence of the real part in order to switch complex conjugations of the first term in the last line such that all variations which carry a complex-conjugation depend on the variable q. In exactly the same way as we did in the proof of the previous Lemma 4.1.8, we now decompose the momentum-space variations by combining (4.3) with the multipole expansions from (4.6). Along with the relation

$$\overline{\widehat{\delta^{(n)}(\bullet)}}(q) = \overline{\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'} \delta^{(n)}(\bullet)_{lm}(q^0,|\vec{q}|)Y_{lm}(\theta_q,\varphi_q)}$$
$$= \sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'} \overline{\delta^{(n)}(\bullet)_{l'm'}(q^0,|\vec{q}|)}(-1)^{m'}Y_{l'(-m')}(\theta_q,\varphi_q)$$
$$= \sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'} \Big[(-1)^{-m'}\overline{\delta^{(n)}(\bullet)_{l'(-m')}(q^0,|\vec{q}|)}\Big]Y_{l'm'}(\theta_q,\varphi_q)$$

where we defined $\tilde{m}' := -m'$ and subsequently replaced $\tilde{m}' \to m'$ in the last equality, we obtain

$$\delta^2\mathcal{L}^\varepsilon(\xi) \underset{(4.9b)}{\overset{(4.7)}{=}} \sum_{l,m}\mathrm{Re}\left\{\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\vec{p}}{(2\pi)^4}\;\mathbb{1}_{1\times5}\mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})(\Delta^2)^\varepsilon_{lm}(|\vec{p}|)\right\}$$
$$+\frac{1}{2}\sum_{\substack{l,m\\ l',m'}}\mathrm{Re}\left\{\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\vec{p}}{(2\pi)^4}\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\vec{q}}{(2\pi)^4}\;\Delta^\varepsilon_{lm}(|\vec{p}|)^{\mathrm{T}}\mathcal{M}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q})\Delta^\varepsilon_{l'm'}(|\vec{q}|)\right\}$$
$$+\frac{1}{2}\sum_{\substack{l,m\\ l',m'}}\mathrm{Re}\left\{\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\vec{p}}{(2\pi)^4}\int_{\mathbb{R}^3}\frac{\mathrm{d}^3\vec{q}}{(2\pi)^4}\;\Delta^\varepsilon_{lm}(|\vec{p}|)^{\mathrm{T}}\mathcal{N}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q})\overline{\Delta^\varepsilon_{l'(-m')}(|\vec{q}|)}\right\}$$

Without explicitly spelling out the individual steps, we have carried out the integrals with respect to p^0 and q^0 and exploited the properties of the δ-distribution together with the assumption that the implicit equation $\sigma^\varepsilon(p^0,|\vec{p}|)=0$ has two regularization-dependent solutions $p^0=\pm\omega^\varepsilon_p$.

By analogy with Lemma 4.1.8, the functions $\mathcal{M}^\varepsilon_{lm|l'm'},\mathcal{N}^\varepsilon_{lm|l'm'}$ for all $(l,m),(l'm')\in\mathbb{N}_0\times\mathbb{Z}$ with $-m^{(\prime)}\le l^{(\prime)}\le m^{(\prime)}$ are given by

$$\mathcal{M}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q}) = \big(\mathcal{C}^\varepsilon_{\mathcal{M}}\odot\Upsilon_{lm|l'm'}+C^\varepsilon\overset{*}{\Upsilon}_{lm|l'm'}\big)E^\varepsilon_{\mathcal{M}}\mathrm{e}^{-\mathrm{i}(\vec{p}+\vec{q})\cdot\vec{\xi}} \tag{4.19a}$$
$$\mathcal{N}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q}) = \big(\mathcal{C}^\varepsilon_{\mathcal{N}}\odot\Upsilon_{lm|l'm'}-B^\varepsilon\overset{*}{\Upsilon}_{lm|l'm'}\big)(-1)^{-m'}E^\varepsilon_{\mathcal{N}}\mathrm{e}^{-\mathrm{i}(\vec{p}-\vec{q})\cdot\vec{\xi}} \tag{4.19b}$$

where the matrices $\mathcal{C}^\varepsilon_{\mathcal{M}},\mathcal{C}^\varepsilon_{\mathcal{N}}:\mathbb{R}^4\to\mathbb{C}^{5\times5}$, referred to as *coefficient matrices corresponding to* $\mathcal{M}^\varepsilon$ *and* $\mathcal{N}^\varepsilon$, respectively, take the form

$$\mathcal{C}^\varepsilon_{\mathcal{M}}(\xi) = \begin{pmatrix} (\overline{v^\varepsilon_0})^2-C^\varepsilon & -\overline{v^\varepsilon}\,\overline{v^\varepsilon_0}\mathbb{1}_{1\times3} & \overline{v^\varepsilon_0}\,\overline{s^\varepsilon} \\ -\overline{v^\varepsilon}\,\overline{v^\varepsilon_0}\mathbb{1}_{3\times1} & \overline{v^\varepsilon}\,\overline{v^\varepsilon}\mathbb{1}_{3\times3} & -\overline{v^\varepsilon}\,\overline{s^\varepsilon}\mathbb{1}_{3\times1} \\ \overline{v^\varepsilon_0}\,\overline{s^\varepsilon} & -\overline{v^\varepsilon}\,\overline{s^\varepsilon}\mathbb{1}_{1\times3} & (\overline{v^\varepsilon})^2 \end{pmatrix} \tag{4.19a,i}$$

$$\mathcal{C}^\varepsilon_{\mathcal{N}}(\xi) = \begin{pmatrix} -|v^\varepsilon_0|^2+B^\varepsilon & -(\overline{v^\varepsilon_0}g^\varepsilon-2v^\varepsilon_0\overline{v^\varepsilon})\mathbb{1}_{1\times3} & \overline{v^\varepsilon_0}s^\varepsilon+2v^\varepsilon_0\overline{s^\varepsilon} \\ -(\overline{v^\varepsilon}\,v^\varepsilon_0-2v^\varepsilon\overline{v^\varepsilon_0})\mathbb{1}_{3\times1} & (\overline{v^\varepsilon}v^\varepsilon-2v^\varepsilon\overline{v^\varepsilon})\mathbb{1}_{3\times3} & -(\overline{v^\varepsilon}\,s^\varepsilon+2v^\varepsilon\overline{s^\varepsilon})\mathbb{1}_{3\times1} \\ v^\varepsilon_0\overline{s^\varepsilon}+2\overline{v^\varepsilon_0}s^\varepsilon & -(v^\varepsilon\overline{s^\varepsilon}+2\overline{v^\varepsilon}s^\varepsilon)\mathbb{1}_{1\times3} & |v^\varepsilon|^2 \end{pmatrix} \tag{4.19b,i}$$

and where the functions $E^\varepsilon_{\mathcal{M}},E^\varepsilon_{\mathcal{N}}:\mathbb{R}\times(\mathbb{R}^+_0)^2\to\mathbb{C}$ are given by

$$E^\varepsilon_{\mathcal{M}}(\xi^0,|\vec{p}|,|\vec{q}|) = \frac{16\mathrm{e}^{\mathrm{i}(p^0+q^0)\xi^0}}{\big|\partial_{p^0}\sigma^\varepsilon(p^0,|\vec{p}|)\big|\big|\partial_{q^0}\sigma^\varepsilon(q^0,|\vec{q}|)\big|}\Bigg|_{\substack{p^0=-\omega^\varepsilon_p\\ q^0=-\omega^\varepsilon_q}} \tag{4.19a,ii}$$

$$E^\varepsilon_{\mathcal{N}}(\xi^0,|\vec{p}|,|\vec{q}|) = \frac{16\mathrm{e}^{\mathrm{i}(p^0-q^0)\xi^0}}{\big|\partial_{p^0}\sigma^\varepsilon(p^0,|\vec{p}|)\big|\big|\partial_{q^0}\sigma^\varepsilon(q^0,|\vec{q}|)\big|}\Bigg|_{\substack{p^0=-\omega^\varepsilon_p\\ q^0=-\omega^\varepsilon_q}} \tag{4.19b,ii}$$

We remark that the asterisked terms $\overset{*}{\Upsilon}_{lm|l'm'}$ arise from those terms in $\delta^2\mathcal{L}^\varepsilon(\xi)$ in which first-order variations of the regularized kernel of the fermionic projector are contracted with each other. □

For the sake of completeness, we shall take the opportunity at this point to introduce, by analogy with $\mathcal{M}^\varepsilon_{lm|l'm'}$ and $\mathcal{N}^\varepsilon_{lm|l'm'}$, two more matrix-valued functions which will become relevant in the following section.

Definition 4.1.10 (Matrix-Valued Functions $\mathcal{V}^\varepsilon_{lm|l'm'}$ and $\mathcal{W}^\varepsilon_{lm|l'm'}$)

The matrix-valued functions $\mathcal{V}^\varepsilon_{lm|l'm'}, \mathcal{W}^\varepsilon_{lm|l'm'} : \mathbb{R}^4 \times (\mathbb{R}^3)^2 \to \mathbb{C}^{5\times 5}$ are defined as

$$\mathcal{V}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q}) \overset{(4.11a)}{=} \frac{1}{2}\frac{\mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})\mathbb{1}_5\,\mathcal{K}^\varepsilon_{l'm'}(\xi,\vec{q})}{\partial_r\mathcal{L}^\varepsilon(\xi)}\bigg|_{r=R^\varepsilon_{\max}(\xi^0)} \tag{4.20a}$$

$$\mathcal{W}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q}) \overset{(4.11a)}{=} \frac{1}{2}\frac{\mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})\mathbb{1}_5\,\overline{\mathcal{K}^\varepsilon_{l'(-m')}(\xi,\vec{q})}}{\partial_r\mathcal{L}^\varepsilon(\xi)}\bigg|_{r=R^\varepsilon_{\max}(\xi^0)} \tag{4.20b}$$

where $R^\varepsilon_{\max}$ denotes the demarcation function as defined in Definition 2.3.8 and $\mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})$ is the matrix-valued function from (4.11a).

4.2 Multipole Expansion of $\delta\mathcal{S}^\varepsilon$ and $\delta^2\mathcal{S}^\varepsilon$

Building on the preliminary work from the previous section, we can now tackle the derivation of the multipole expansion of the variations $\delta\mathcal{S}^\varepsilon$ and $\delta^2\mathcal{S}^\varepsilon$. For this, we have to insert the multipole expansions of $\delta\mathcal{L}^\varepsilon(\xi)$ and $\delta^2\mathcal{L}^\varepsilon(\xi)$ as derived in Lemma 4.1.8 and Lemma 4.1.9 into the expressions for $\delta\mathcal{S}^\varepsilon$ and $\delta^2\mathcal{S}^\varepsilon$ from Theorem 3.4.3. By interchanging the position space integral over the region $\mathcal{R}^\varepsilon$ (coming from the causal action) with the momentum space integrals (coming from the Fourier decomposition of $\delta\mathcal{L}^\varepsilon(\xi)$ and $\delta^2\mathcal{L}^\varepsilon(\xi)$) and recalling that the Fourier exponential factors are included in the matrix-valued functions $\mathcal{K}^\varepsilon_{lm}$, $\mathcal{M}^\varepsilon_{lm|l'm'}$, $\mathcal{N}^\varepsilon_{lm|l'm'}$, $\mathcal{V}^\varepsilon_{lm|l'm'}$ $\mathcal{W}^\varepsilon_{lm|l'm'}$ it will turn out to be advantageous to introduce so-called *incomplete Fourier transforms*.

Definition 4.2.1 (Incomplete Fourier Transforms)

The *incomplete Fourier transforms* of the matrix-valued functions $\mathcal{K}^\varepsilon_{lm}$, $\mathcal{M}^\varepsilon_{lm|l'm'}$ and $\mathcal{N}^\varepsilon_{lm|l'm'}$ as introduced in (4.11a), (4.17a) and (4.17b), respectively, are defined as

$$\mathcal{F}\big[\mathcal{K}^\varepsilon_{lm}\big](\vec{p}) \overset{(4.11a)}{=} \int_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0,r) \int_{S^2} \mathrm{d}\Omega_\xi\; r^2\mathcal{K}^\varepsilon_{lm}(\xi,\vec{p}) \tag{4.21a}$$

$$\begin{Bmatrix} \mathcal{F}\big[\mathcal{M}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) \\ \mathcal{F}\big[\mathcal{N}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) \end{Bmatrix} \overset{(4.17a)}{\underset{(4.17b)}{=}} \int_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0,r) \int_{S^2} \mathrm{d}\Omega_\xi\; r^2 \begin{Bmatrix} \mathcal{M}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q}) \\ \mathcal{N}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q}) \end{Bmatrix} \tag{4.21b}$$

where we have decomposed the domain of integration $\mathcal{R}^\varepsilon$ as $\mathcal{R}^\varepsilon = \mathcal{X}^\varepsilon \times S^2$. Likewise, for the functions $\mathcal{V}^\varepsilon_{lm|l'm'}$ and $\mathcal{W}^\varepsilon_{lm|l'm'}$ as introduced in (4.20a) and (4.20b), the incomplete Fourier transforms are defined as

$$\begin{Bmatrix} \mathcal{F}\big[\mathcal{V}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) \\ \mathcal{F}\big[\mathcal{W}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) \end{Bmatrix} \overset{(4.20a)}{\underset{(4.20b)}{=}} \int_{\mathbb{R}} \mathrm{d}\xi^0 \int_{S^2} \mathrm{d}\Omega_\xi\; R^\varepsilon_{\max}(\xi^0)^2 \begin{Bmatrix} \mathcal{V}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q}) \\ \mathcal{W}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q}) \end{Bmatrix}\bigg|_{r=R^\varepsilon_{\max}(\xi^0)} \tag{4.21c}$$

Let us remark that the terminology *incomplete Fourier transforms* reflects the fact that the radial integrals do not extend to infinity as would be the case for ordinary Fourier transforms (in spherical coordinates). This can ultimately be traced back to the fact that the homogeneous regularized causal Lagrangian $\mathcal{L}^\varepsilon_{\mathrm{h}}(\xi)$ vanishes for $\xi \in \mathbb{R}^4 \setminus \mathcal{R}^\varepsilon$. Using these incomplete Fourier transforms, the multipole expansions of the variations of the regularized causal action take the following form.

Lemma 4.2.2 (Multipole Expansion of $\delta\mathcal{S}^\varepsilon$ and $\delta^2\mathcal{S}^\varepsilon$)

The multipole moments in the expansions $\delta\mathcal{S}^\varepsilon = \sum_{l,m} \delta\mathcal{S}^\varepsilon_{lm}$ and $\delta^2\mathcal{S}^\varepsilon = \sum_{l,m,l',m'} \delta^2\mathcal{S}^\varepsilon_{lm|l'm'}$, expressed in terms of the incomplete Fourier transforms (4.21), are given by

$$\delta\mathcal{S}^\varepsilon_{lm} = \mathrm{Re}\left\{ \int\limits_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}}{(2\pi)^4}\; \mathbb{1}_{1\times 5}\,\mathcal{F}\big[\mathcal{K}^\varepsilon_{lm}\big](\vec{p})\Delta^\varepsilon_{lm}(|\vec{p}\,|) \right\} \tag{4.22a}$$

and

$$\begin{aligned}\delta^2\mathcal{S}^\varepsilon_{lm|l'm'} = \mathrm{Re}\Bigg\{ &\int\limits_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}}{(2\pi)^4}\; \delta_{ll'}\delta_{mm'}\mathbb{1}_{1\times 5}\,\mathcal{F}\big[\mathcal{K}^\varepsilon_{lm}\big](\vec{p})(\Delta^2)^\varepsilon_{lm}(|\vec{p}\,|) + \frac{1}{2}\int\limits_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}}{(2\pi)^4} \int\limits_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{q}}{(2\pi)^4} \times \\ &\times \Delta^\varepsilon_{lm}(|\vec{p}\,|)^{\mathrm{T}} \Big[(-1)^{m'}\mathcal{F}\big[\mathcal{M}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) - (-1)^{m'}\mathcal{F}\big[\mathcal{V}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) \\ &\qquad + \mathcal{F}\big[\mathcal{N}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) - \mathcal{F}\big[\mathcal{W}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q})\Big]\overline{\Delta^\varepsilon_{l'(-m')}(|\vec{q}\,|)} \Bigg\}\end{aligned} \tag{4.22b}$$

respectively.

Proof. We proceed in two steps and start with the derivation of the multipole expansion of $\delta\mathcal{S}^\varepsilon$.

(1) Multipole Expansion of $\delta\mathcal{S}^\varepsilon$

Inserting for $\delta\mathcal{L}^\varepsilon(\xi)$ in (3.31a) the multipole expansion as given in (4.11) and interchanging the momentum and position space integrals using Fubini's theorem, we obtain

$$\begin{aligned}\delta\mathcal{S}^\varepsilon &\overset{(3.31a)}{=} \int\limits_{\mathbb{R}} \mathrm{d}\xi^0 \int\limits_{S^2} \mathrm{d}\Omega_\xi \int\limits_0^{R^\varepsilon_{\max}(\xi^0)} \mathrm{d}r\; r^2 \delta\mathcal{L}^\varepsilon(\xi) \\ &\overset{(4.11)}{=} \sum_{l,m} \mathrm{Re}\left\{ \int\limits_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}}{(2\pi)^4} \int\limits_{\mathbb{R}} \mathrm{d}\xi^0 \int\limits_0^{R^\varepsilon_{\max}(\xi^0)} \mathrm{d}r \int\limits_{S^2} \mathrm{d}\Omega_\xi\; \mathbb{1}_{1\times 5} r^2 \mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})\Delta^\varepsilon_{lm}(|\vec{p}\,|) \right\}\end{aligned}$$

Combing the ξ^0-integral and the radial integral and employing the definition of the incomplete Fourier transform of the matrix-valued function $\mathcal{K}^\varepsilon_{lm}$ which was introduced in (4.21a), we find

$$\delta\mathcal{S}^\varepsilon \overset{(4.21a)}{=} \sum_{l,m} \mathrm{Re}\left\{ \int\limits_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}}{(2\pi)^4}\; \mathbb{1}_{1\times 5}\,\mathcal{F}\big[\mathcal{K}^\varepsilon_{lm}\big](\vec{p})\Delta^\varepsilon_{lm}(|\vec{p}\,|) \right\} \tag{4.23}$$

which concludes the proof for the multipole expansion of $\delta\mathcal{S}^\varepsilon$.

(2) Multipole Expansion of $\delta^2\mathcal{S}^\varepsilon$

For the derivation of the multipole expansion of $\delta^2\mathcal{S}^\varepsilon$ the approach is basically the same as for $\delta\mathcal{S}^\varepsilon$, though slightly more involved. Inserting for $\delta\mathcal{L}^\varepsilon(\xi)$ and $\delta^2\mathcal{L}^\varepsilon(\xi)$ in (3.31b) the multipole expansions as given in (4.11) and (4.17), respectively, we obtain

$$\delta^2\mathcal{S}^\varepsilon \overset{(3.31b)}{=} \int_{\mathbb{R}} d\xi^0 \int_{S^2} d\Omega_\xi \left[\int_0^{R^\varepsilon_{\max}(\xi^0)} dr\ r^2 \delta^2\mathcal{L}^\varepsilon(\xi) - \frac{1}{2}\left(r^2 \frac{\delta\mathcal{L}^\varepsilon(\xi)^2}{\partial_r \mathcal{L}^\varepsilon(\xi)}\right)\bigg|_{r=R^\varepsilon_{\max}(\xi^0)} \right]$$

$$\overset{(4.17)}{\underset{(4.11)}{=}} \sum_{l,m} \mathrm{Re}\Bigg\{ \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^4} \int_{\mathbb{R}} d\xi^0 \int_0^{R^\varepsilon_{\max}(\xi^0)} dr \int_{S^2} d\Omega_\xi\ r^2 \mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})(\Delta^2)^\varepsilon_{lm}(|\vec{p}|)$$

$$+ \frac{1}{2}\sum_{l',m'} \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^4} \int_{\mathbb{R}^3} \frac{d^3\vec{q}}{(2\pi)^4} \int_{\mathbb{R}} d\xi^0 \int_0^{R^\varepsilon_{\max}(\xi^0)} dr \int_{S^2} d\Omega_\xi \times$$

$$\times\, r^2 \Big(\Delta^\varepsilon_{lm}(|\vec{p}|)^{\mathrm{T}} \mathcal{M}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q}) \Delta^\varepsilon_{l'm'}(|\vec{q}|) + \Delta^\varepsilon_{lm}(|\vec{p}|)^{\mathrm{T}} \mathcal{N}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q}) \overline{\Delta^\varepsilon_{l'(-m')}(|\vec{q}|)} \Big)$$

$$- \frac{1}{4}\sum_{l',m'} \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^4} \int_{\mathbb{R}^3} \frac{d^3\vec{q}}{(2\pi)^4} \int_{\mathbb{R}} d\xi^0 \int_{S^2} d\Omega_\xi \left[\frac{r^2}{\partial_r \mathcal{L}^\varepsilon(\xi)} \times \right.$$

$$\left.\left. \times \Big(\mathbb{1}_{1\times5}\, \mathcal{K}^\varepsilon_{lm}(\xi,\vec{p}) \Delta^\varepsilon_{lm}(|\vec{p}|) \mathbb{1}_{1\times5}\, \mathcal{K}^\varepsilon_{l'm'}(\xi,\vec{q}) \Delta^\varepsilon_{l'm'}(|\vec{q}|) + \mathbb{1}_{1\times5}\, \mathcal{K}^\varepsilon_{lm}(\xi,\vec{p}) \Delta^\varepsilon_{lm}(|\vec{p}|) \overline{\mathbb{1}_{1\times5}\, \mathcal{K}^\varepsilon_{l'm'}(\xi,\vec{q}) \Delta^\varepsilon_{l'm'}(|\vec{q}|)} \Big) \right] \right|_{r=R^\varepsilon_{\max}(\xi^0)} \Bigg\}$$

For the term containing the inverse of the radial derivative of the regularized causal Lagrangian we made use of the relation $\mathrm{Re}(x)^2 = \frac{1}{2}\mathrm{Re}(x^2 + |x|^2)$ which leads to the appearance of an additional factor $\frac{1}{2}$. By exploiting the fact that $\mathbb{1}_{1\times5}\, \mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})\Delta_{lm}(|\vec{p}|)$ is scalar-valued and thus invariant under transposition, the integrands in the last two lines can be rewritten as

$$\begin{aligned} &\mathbb{1}_{1\times5}\mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})\Delta^\varepsilon_{lm}(|\vec{p}|)\mathbb{1}_{1\times5}\mathcal{K}^\varepsilon_{l'm'}(\xi^\varepsilon,\vec{q})\Delta^\varepsilon_{l'm'}(|\vec{q}|) = \\ &\quad = \big(\mathbb{1}_{1\times5}\mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})\Delta^\varepsilon_{lm}(|\vec{p}|)\big)^{\mathrm{T}} \mathbb{1}_{1\times5}\mathcal{K}^\varepsilon_{l'm'}(\xi^\varepsilon,\vec{q})\Delta^\varepsilon_{l'm'}(|\vec{q}|) \\ &\quad = \Delta^\varepsilon_{lm}(|\vec{p}|)^{\mathrm{T}}\mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})^{\mathrm{T}}\mathbb{1}_5\mathcal{K}^\varepsilon_{l'm'}(\xi,\vec{q})\Delta^\varepsilon_{l'm'}(|\vec{q}|) \end{aligned}$$

and

$$\begin{aligned} &\sum_{l',m'} \mathbb{1}_{1\times5}\, \mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})\Delta^\varepsilon_{lm}(|\vec{p}|)\overline{\mathbb{1}_{1\times5}\, \mathcal{K}^\varepsilon_{l'm'}(\xi,\vec{q})}\, \overline{\Delta^\varepsilon_{l'm'}(|\vec{q}|)} = \\ &\quad = \sum_{l',m'} \big(\mathbb{1}_{1\times5}\mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})\Delta^\varepsilon_{lm}(|\vec{p}|)\big)^{\mathrm{T}} \overline{\mathbb{1}_{1\times5}\, \mathcal{K}^\varepsilon_{l'm'}(\xi,\vec{q})}\, \overline{\Delta^\varepsilon_{l'm'}(|\vec{q}|)} \\ &\quad = \sum_{l',m'} \Delta^\varepsilon_{lm}(|\vec{p}|)^{\mathrm{T}}\mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})^{\mathrm{T}}\mathbb{1}_5\, \overline{\mathcal{K}^\varepsilon_{l'(-m')}(\xi,\vec{q})}\, \overline{\Delta^\varepsilon_{l'(-m')}(|\vec{q}|)} \end{aligned}$$

where we defined $\tilde{m}' := -m'$ and subsequently replaced $\tilde{m}' \to m'$ in the last equality. Recalling that $\mathcal{K}^\varepsilon_{lm}$ is a diagonal matrix (and thus invariant under transposition) and expressing the above combination of matrices $\mathcal{K}^\varepsilon_{lm}$ and $\mathcal{K}^\varepsilon_{l'm'}$ in terms of the matrices $\mathcal{V}^\varepsilon_{lm|l'm'}$ and $\mathcal{W}^\varepsilon_{lm|l'm'}$ introduced in (4.20), we arrive at

$$\delta^2\mathcal{S}^\varepsilon \overset{(4.20)}{=} \sum_{\substack{l,m\\ l',m'}} \mathrm{Re}\Bigg\{ \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^4} \int_{\mathcal{X}^\varepsilon} d(\xi^0,r) \int_{S^2} d\Omega_\xi\ \delta_{ll'}\delta_{mm'} r^2 \mathbb{1}_{1\times5}\, \mathcal{K}^\varepsilon_{lm}(\xi,\vec{p})(\Delta^2)^\varepsilon_{lm}(|\vec{p}|)$$

$$+ \frac{1}{2} \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^4} \int_{\mathbb{R}^3} \frac{d^3\vec{q}}{(2\pi)^4} \int_{\mathcal{X}^\varepsilon} d(\xi^0,r) \int_{S^2} d\Omega_\xi\ r^2 \Big(\Delta^\varepsilon_{lm}(|\vec{p}|)^{\mathrm{T}} \mathcal{M}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q}) \Delta^\varepsilon_{l'm'}(|\vec{q}|) + \Delta^\varepsilon_{lm}(|\vec{p}|)^{\mathrm{T}} \mathcal{N}^\varepsilon_{lm|l'm'}(\xi,\vec{p},\vec{q}) \overline{\Delta^\varepsilon_{l'(-m')}(|\vec{q}|)} \Big)$$

$$- \frac{1}{2} \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^4} \int_{\mathbb{R}^3} \frac{d^3\vec{q}}{(2\pi)^4} \int_{\mathbb{R}} d\xi^0 \int_{S^2} d\Omega_\xi \; R^\varepsilon_{\max}(\xi^0)^2 \Big(\Delta^\varepsilon_{lm}(|\vec{p}|) \mathcal{V}^\varepsilon_{lm|l'm'}(\xi, \vec{p}, \vec{q}) \Delta^\varepsilon_{l'm'}(|\vec{q}|) + \Delta^\varepsilon_{lm}(|\vec{p}|) \mathcal{W}^\varepsilon_{lm|l'm'}(\xi, \vec{p}, \vec{q}) \overline{\Delta^\varepsilon_{l'(-m')}(|\vec{q}|)} \Big) \Bigg\}$$

Inserting the definition of the incomplete Fourier transforms from Definition 4.2.1 and replacing $\Delta^\varepsilon_{l'm'}$ by $(-1)^{m'} \overline{\Delta^\varepsilon_{l'(-m')}}$ by exploiting the symmetry properties of the spherical harmonics along with the fact that variations of the regularized kernel of the fermionic projector in momentum space are real-valued, results in

$$\delta^2 \mathcal{S}^\varepsilon \overset{(4.21)}{=} \sum_{\substack{l,m\\ l',m'}} \mathrm{Re} \Bigg\{ \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^4} \; \delta_{ll'} \delta_{mm'} \mathbb{1}_{1\times 5} \, \mathcal{F}\big[\mathcal{K}^\varepsilon_{lm}\big](\vec{p}) (\Delta^2)^\varepsilon_{lm}(|\vec{p}|) + \frac{1}{2} \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^4} \int_{\mathbb{R}^3} \frac{d^3\vec{q}}{(2\pi)^4} \times \\ \times \Big[\Delta^\varepsilon_{lm}(|\vec{p}|)^{\mathrm{T}} \Big((-1)^{m'} \mathcal{F}\big[\mathcal{M}^\varepsilon_{lm|l'm'}\big](\vec{p}, \vec{q}) - (-1)^{m'} \mathcal{F}\big[\mathcal{V}^\varepsilon_{lm|l'm'}\big](\vec{p}, \vec{q}) + \mathcal{F}\big[\mathcal{N}^\varepsilon_{lm|l'm'}\big](\vec{p}, \vec{q}) - \mathcal{F}\big[\mathcal{W}^\varepsilon_{lm|l'm'}\big](\vec{p}, \vec{q}) \Big) \overline{\Delta^\varepsilon_{l'(-m')}(|\vec{q}|)} \Big] \Bigg\}$$

By analogy with Lemma 4.1.9, the matrix-valued functions $\mathcal{V}^\varepsilon_{lm|l'm'}(\xi, \vec{p}, \vec{q})$ and $\mathcal{W}^\varepsilon_{lm|l'm'}(\xi, \vec{p}, \vec{q})$ introduced in (4.20) can each be decomposed into a Hadamard product of coefficient matrices $\mathcal{C}^\varepsilon_{\mathcal{V}}, \mathcal{C}^\varepsilon_{\mathcal{W}} : \mathbb{R}^4 \to \mathbb{C}^{5\times 5}$ with the matrix $\Upsilon_{lm|l'm'}$ from (4.20) as

$$\mathcal{V}^\varepsilon_{lm|l'm'}(\xi, \vec{p}, \vec{q}) = \big[\mathcal{C}^\varepsilon_{\mathcal{V}} \odot \Upsilon_{lm|l'm'}\big] E^\varepsilon_{\mathcal{V}} e^{-i(\vec{p}+\vec{q})\cdot\vec{\xi}} \tag{4.24a}$$

$$\mathcal{W}^\varepsilon_{lm|l'm'}(\xi, \vec{p}, \vec{q}) = \big[\mathcal{C}^\varepsilon_{\mathcal{W}} \odot \Upsilon_{lm|l'm'}\big] (-1)^{-m'} E^\varepsilon_{\mathcal{W}} e^{-i(\vec{p}-\vec{q})\cdot\vec{\xi}} \tag{4.24b}$$

where the functions $E^\varepsilon_{\mathcal{V}}$ and $E^\varepsilon_{\mathcal{W}}$ are defined as

$$E^\varepsilon_{\mathcal{V}}(\xi^0, |\vec{p}|, |\vec{q}|) := \frac{1}{2} \frac{E^\varepsilon_{\mathcal{K}}(\xi^0, |\vec{p}|) E^\varepsilon_{\mathcal{K}}(\xi^0, |\vec{q}|)}{\partial_r \mathcal{L}^\varepsilon(\xi)} \bigg|_{r = R^\varepsilon_{\max}(\xi^0)} \tag{4.24a,i}$$

$$E^\varepsilon_{\mathcal{W}}(\xi^0, |\vec{p}|, |\vec{q}|) := \frac{1}{2} \frac{E^\varepsilon_{\mathcal{K}}(\xi^0, |\vec{p}|) \overline{E^\varepsilon_{\mathcal{K}}(\xi^0, |\vec{q}|)}}{\partial_r \mathcal{L}^\varepsilon(\xi)} \bigg|_{r = R^\varepsilon_{\max}(\xi^0)} \tag{4.24b,i}$$

To arrive at the above Hadamard product form of the matrices $\mathcal{V}^\varepsilon_{lm|l'm'}$ and $\mathcal{W}^\varepsilon_{lm|l'm'}$, we used the fact that a matrix product $(D_v \odot D_w)\mathbb{1}_n(D_x \odot D_y)$ with diagonal $(n \times n)$-matrices D_v corresponding to n-component vectors v can be rewritten as follows

$$\begin{aligned}
\big[(D_v \odot D_w)\mathbb{1}_n(D_x \odot D_y)\big]_{ij} &= \big[(D_v \odot D_w)(\mathbb{1}_n \odot \mathbb{1}_n)(D_x \odot D_y)\big]_{ij} \\
&= (D_v \odot D_w)_{ik}(\mathbb{1}_n \odot \mathbb{1}_n)_{kl}(D_x \odot D_y)_{lj} \\
&= (D_v)_{ii}(D_w)_{ii}\delta_{ik}(\mathbb{1}_n)_{kl}(\mathbb{1}_n)_{kl}(D_x)_{jj}(D_y)_{jj}\delta_{lj} \\
&= (D_v)_{ii}(\mathbb{1}_n)_{ij}(D_x)_{jj}(D_w)_{ii}(\mathbb{1}_n)_{ij}(D_y)_{jj} \\
&= (D_v)_{ii}\delta_{ki}(\mathbb{1}_n)_{kl}\delta_{lj}(D_x)_{jj}(D_w)_{ii}\delta_{ri}(\mathbb{1}_n)_{rs}\delta_{sj}(D_y)_{jj} \\
&= \big[(D_v)_{ik}(\mathbb{1}_n)_{kl}(D_x)_{lj}\big]\big[(D_w)_{ir}(\mathbb{1}_n)_{rs}(D_y)_{sj}\big] \\
&= \big[\big(D_v\mathbb{1}_n D_x\big) \odot \big(D_w \mathbb{1}_n D_y\big)\big]_{ij}
\end{aligned}$$

Applying this result to the matrices defined in (4.20) by identifying the diagonal matrices as $D_v, D_x \equiv \mathcal{C}_{\mathcal{K}}$, $D_w \equiv \Upsilon_{lm}$, $D_y \equiv \Upsilon_{l'm'}$, we are let to defining

$$\mathcal{C}^\varepsilon_{\mathcal{V}} := \mathcal{C}^\varepsilon_{\mathcal{K}} \mathbb{1}_5 \mathcal{C}^\varepsilon_{\mathcal{K}} \big|_{r = R^\varepsilon_{\max}(\xi^0)} \tag{4.24a,ii}$$

$$\mathcal{C}^\varepsilon_{\mathcal{W}} := \mathcal{C}^\varepsilon_{\mathcal{K}} \mathbb{1}_5 \overline{\mathcal{C}^\varepsilon_{\mathcal{K}}} \big|_{r = R^\varepsilon_{\max}(\xi^0)} \tag{4.24b,ii}$$

which, together with the relation $\Upsilon_{lm|l'm'} = \Upsilon_{lm}\mathbb{1}_5\Upsilon_{l'm'}$, concludes the proof. □

Having reached this point, we shall pause for a moment to place what has been achieved so far in the larger context and to explain the next steps: As mentioned at the beginning of this chapter as well as in the paragraph on the optimization of the regularization, the multipole expansions of $\delta\mathcal{S}^\varepsilon$ and $\delta^2\mathcal{S}^\varepsilon$ provide information on how anisotropic deformations of the regularization affect the regularized causal action. In order to make this information accessible and to investigate whether there are, for example, deformations that leave the regularized causal action invariant, the remaining part of this chapter is concerned with simplifying the expressions for $\delta\mathcal{S}^\varepsilon$ and $\delta^2\mathcal{S}^\varepsilon$ obtained in the previous Lemma 4.2.2 by first performing the angular integrals in position space in Subsection 4.2.1, before we also compute the momentum space angular integrals in Subsection 4.2.2 which ultimately results in Theorem 4.3.1.

Procedural Note Due to the fact that the following computations are lengthy and unwieldy, but nevertheless important, we have outsourced them, graded according to their rank of importance as lemmas, propositions and auxiliary calculations, to Appendix C and just kept the most important steps and results as lemmas in the main body. As a consequence of this approach, the proofs of these lemmas are rather short and text-intensive by only stating the main idea and referring to (combinations of) propositions for the full calculations including all details.

4.2.1 Performing the Position Space Angular Integration

We start the simplification procedure by carrying out the position space angular integrals contained in the incomplete Fourier transforms as given in (4.21a), (4.21b) and (4.21c). Due to the fact that the regularization of the *unperturbed* kernel of the fermionic projector is assumed to be spherically symmetric, the only dependence of the integrands of the incomplete Fourier transforms on the position space angular variables enters via the Fourier exponentials contained in the functions $E^\varepsilon_\bullet$. As a consequence, the coefficient matrices $\mathfrak{C}^\varepsilon_\bullet$ whose entries are combinations of the components of the regularized kernel of the fermionic projector, do not play a role in the computation of these integrals. Before we start with the explicit calculations, we introduce the following definition.

Definition 4.2.3 (Generalized Spherical Bessel Functions)

For any $n \in \mathbb{Z}$ the functions $j_{0,n}$, which will be referred to as *generalized spherical Bessel functions*, are defined as

$$j_{0,n}(x) := \frac{j_0(x)}{x^{n-1}} \tag{4.26}$$

where $j_0(x) = \mathrm{sinc}(x)$ denotes the first spherical Bessel function.

In order to evaluate the position space angular integrals in the incomplete Fourier transforms, we make use of the following proposition.

Proposition 4.2.4 (Position Space Angular Integration of Υ_{lm}, $\Upsilon_{lm|l'm'}$, $\overset{*}{\Upsilon}_{lm|l'm'}$)

Let $h, k \in C^1(\mathbb{R}^+_0, \mathbb{R})$. Then, when integrated on both sides against $h(|\vec{p}|)$ and $h(|\vec{p}|)k(|\vec{q}|)$ over $\mathbb{R}^3$ and $\mathbb{R}^3 \times \mathbb{R}^3$, respectively, the following equalities hold

$$\int_{S^2} \mathrm{d}\Omega_\xi \; \Upsilon_{lm} \mathrm{e}^{-\mathrm{i}\vec{p}\cdot\vec{\xi}} \overset{(C.39)}{=} Y_{lm} \times \mathfrak{k}^{(1)} j_{0,1}(|\vec{p}|r) \tag{4.27a}$$

$$\int_{S^2} \mathrm{d}\Omega_\xi \; \Upsilon_{lm|l'm'} \mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} \underset{(C.39)}{\overset{(C.32)}{=}} Y_{lm} Y_{l'm'} \times \sum_{\substack{n=-1 \\ n \text{ odd}}}^{5} \begin{cases} \mathfrak{m}^{(n)} j_{0,n}(|\vec{p}+\vec{q}|r) & \text{for } \vec{p}+\vec{q} \\ \mathfrak{n}^{(n)} j_{0,n}(|\vec{p}-\vec{q}|r) & \text{for } \vec{p}-\vec{q} \end{cases} \tag{4.27b}$$

$$\int_{S^2} \mathrm{d}\Omega_\xi \;\, \overset{*}{\Upsilon}_{lm|l'm'} \mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} \overset{\text{(C.51)}}{=} Y_{lm} Y_{l'm'} \times \sum_{\substack{n=1 \\ n \text{ odd}}}^{5} \begin{cases} \overset{*}{\mathfrak{m}}^{(n)} j_{0,n}(|\vec{p}+\vec{q}|r) & \text{for } \vec{p}+\vec{q} \\ \overset{*}{\mathfrak{n}}^{(n)} j_{0,n}(|\vec{p}-\vec{q}|r) & \text{for } \vec{p}-\vec{q} \end{cases} \tag{4.27c}$$

where $\mathfrak{k}^{(1)}$ and $\mathfrak{m}^{(n)}$, $\mathfrak{n}^{(n)}$, $\overset{*}{\mathfrak{m}}^{(n)}$, $\overset{*}{\mathfrak{n}}^{(n)}$ for $n \in \{-1, 1, 3, 5\}$ denote the matrix-valued differential operators with respect to r which are explicitly given in Definition C.4.2.

Proof. As the proof of these relations is rather lengthy, we only sketch the basic idea using the example of (4.27b) and refer to Appendix Sections C.2 to C.4 for the full calculations including all details.

Multiplying the left-hand side of (4.27b) with $h(|\vec{p}|)k(|\vec{q}|)$, integrating over $\mathbb{R}^3 \times \mathbb{R}^3$ and inserting the definition of the matrix $\Upsilon_{lm|l'm'}$ from (4.9b) yields

$$\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \int_{S^2} \mathrm{d}\Omega_\xi \begin{pmatrix} Y_{lm}Y_{l'm'} & Y_{lm}\xi^\beta \begin{bmatrix} Y^\beta_{l'm'} & \Psi^\beta_{l'm'} & \Phi^\beta_{l'm'} \end{bmatrix} & Y_{lm}Y_{l'm'} \\ \xi^\alpha \begin{bmatrix} Y^\alpha_{lm} \\ \Psi^\alpha_{lm} \\ \Phi^\alpha_{lm} \end{bmatrix} Y_{l'm'} & \xi^\alpha\xi^\beta \begin{bmatrix} Y^\alpha_{lm}Y^\beta_{l'm'} & Y^\alpha_{lm}\Psi^\beta_{l'm'} & Y^\alpha_{lm}\Phi^\beta_{l'm'} \\ \Psi^\alpha_{lm}Y^\beta_{l'm'} & \Psi^\alpha_{lm}\Psi^\beta_{l'm'} & \Psi^\alpha_{lm}\Phi^\beta_{l'm'} \\ \Phi^\alpha_{lm}Y^\beta_{l'm'} & \Phi^\alpha_{lm}\Psi^\beta_{l'm'} & \Phi^\alpha_{lm}\Phi^\beta_{l'm'} \end{bmatrix} & \xi^\alpha \begin{bmatrix} Y^\alpha_{lm} \\ \Psi^\alpha_{lm} \\ \Phi^\alpha_{lm} \end{bmatrix} Y_{l'm'} \\ Y_{lm}Y_{l'm'} & Y_{lm}\xi^\beta \begin{bmatrix} Y^\beta_{l'm'} & \Psi^\beta_{l'm'} & \Phi^\beta_{l'm'} \end{bmatrix} & Y_{lm}Y_{l'm'} \end{pmatrix} \mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} \tag{4.28}$$

To evaluate the expression, we make use of the block matrix structure introduced in Terminology 4.1.7 and compute the integrals for the dotted, double-dotted and asterisked terms separately which is done in Appendix Section C.2, Appendix Section C.3 and Appendix Section C.4, respectively. The result for the matrix Υ_{lm} follows from Corollary C.2.2 to Lemma C.2.1.

Having decomposed the matrices in this way, the central idea underlying all calculations is to convert derivatives in momentum space (which enter through the vector spherical harmonics) into derivatives with respect to the position space variable r. We achieve this by first rewriting scalar products of $\vec{\xi}$ with vector spherical harmonics as gradients of the exponential factor with respect to the momentum space variables. Subsequently, the position space angular integrals can be easily carried out using Proposition C.1.1 which leads to the appearance of generalized spherical Bessel functions. Afterwards, the momentum space gradients contained in the vector spherical harmonics are converted into position space derivatives with respect to the radial variable r by repeated integration by parts. Finally, the derivatives acting on the generalized spherical Bessel functions are combined into matrix-valued differential operators $\mathfrak{m}^{(n)}$, $\mathfrak{n}^{(n)}$ and $\overset{*}{\mathfrak{m}}^{(n)}$, $\overset{*}{\mathfrak{n}}^{(n)}$ (see Definition C.4.2). □

This proposition now allows to express the incomplete Fourier transforms from Definition 4.2.1 as a product of *scalar* spherical harmonics and regularization-dependent, matrix-valued functions which exclusively depend on the momentum space variables $|\vec{p}|$, $|\vec{q}|$ as well as on $k_\pm := |\vec{p} \pm \vec{q}|$.

Lemma 4.2.5 (Position Space Angular Integration in (4.21))

By carrying out the position space angular integrals using Proposition 4.2.4, the incomplete Fourier transforms as introduced in Definition 4.2.1 evaluate to

$$\mathcal{F}\big[\mathcal{K}^\varepsilon_{lm}\big](\vec{p}) = \int_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0, r)\;\, r^2 Y_{lm} \times E^\varepsilon_{\mathcal{K}}\big(\mathcal{C}^\varepsilon_{\mathcal{K}} \odot \mathfrak{k}^{(1)}\big) j_{0,1}(|\vec{p}|r) \tag{4.29a}$$

$$\begin{Bmatrix} \mathcal{F}\big[\mathcal{M}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) \\ \mathcal{F}\big[\mathcal{N}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) \end{Bmatrix} = \sum_{\substack{n=-1 \\ n \text{ odd}}}^{5} \int_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0, r)\;\, r^2 Y_{lm} Y_{l'm'} \times$$
$$\times \begin{Bmatrix} E^\varepsilon_{\mathcal{M}}\big(\mathcal{C}^\varepsilon_{\mathcal{M}} \odot \mathfrak{m}^{(n)} + C^\varepsilon \overset{*}{\mathfrak{m}}^{(n)}\big) j_{0,n}(k_+ r) \\ (-1)^{-m'} E^\varepsilon_{\mathcal{N}}\big(\mathcal{C}^\varepsilon_{\mathcal{N}} \odot \mathfrak{n}^{(n)} - B^\varepsilon \overset{*}{\mathfrak{n}}^{(n)}\big) j_{0,n}(k_- r) \end{Bmatrix} \tag{4.29b}$$

$$\begin{Bmatrix} \mathcal{F}\big[\mathcal{V}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) \\ \mathcal{F}\big[\mathcal{W}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) \end{Bmatrix} = \sum_{\substack{n=1 \\ n \text{ odd}}}^{5} \int_{\mathbb{R}} \mathrm{d}\xi^0 \; R^\varepsilon_{\max}(\xi^0)^2 Y_{lm} Y_{l'm'} \times \\ \times \begin{Bmatrix} E^\varepsilon_{\mathcal{V}}\big(\mathcal{C}^\varepsilon_{\mathcal{V}} \odot \mathfrak{m}^{(n)}\big) j_{0,n}(k_+ r) \\ (-1)^{-m'} E^\varepsilon_{\mathcal{W}}\big(\mathcal{C}^\varepsilon_{\mathcal{W}} \odot \mathfrak{n}^{(n)}\big) j_{0,n}(k_- r) \end{Bmatrix}\Bigg|_{r=R^\varepsilon_{\max}(\xi^0)} \tag{4.29c}$$

where $\mathcal{C}^\varepsilon_\bullet$ denote the coefficient matrices (see (4.13a), (4.19a,i), (4.19b,i), (4.24a,ii), (4.24b,ii)), $E^\varepsilon_\bullet$ the corresponding functions containing the exponential factor as well as the regularization of the mass shell (see (4.13b), (4.19a,ii), (4.19b,ii), (4.24a,i), (4.24b,i)) and $\mathfrak{m}^{(n)}$, $\mathfrak{n}^{(n)}$, $\mathring{\mathfrak{m}}^{(n)}$, $\mathring{\mathfrak{n}}^{(n)}$ stand for the matrix-valued differential operators as introduced in Definition C.4.2.

Proof. The assumption of spherical symmetry for the regularization of the unperturbed kernel of the fermionic projector implies that within the matrix-valued functions $\mathcal{K}^\varepsilon_{lm}$, $\mathcal{M}^\varepsilon_{lm|l'm'}$, $\mathcal{N}^\varepsilon_{lm|l'm'}$, $\mathcal{V}^\varepsilon_{lm|l'm'}$, $\mathcal{W}^\varepsilon_{lm|l'm'}$ only the Fourier exponentials (which are contained in the functions $E^\varepsilon_\bullet$) as well as the matrices of spherical harmonics Υ_{lm} and $\Upsilon_{lm|l'm'}$ depend on position space angular variables. As a consequence of this, the position space angular integrals in Definition 4.2.1 can be carried out using Proposition 4.2.4 while the coefficient matrices $\mathcal{C}^\varepsilon_\bullet$ as well as the functions B^ε and C^ε remain unchanged. □

4.2.2 Performing the Momentum Space Angular Integrations

Having completed the computation of the position space angular integrals contained in the incomplete Fourier transforms in the previous subsection, we have already come one big step closer to our goal, namely to simplify the expressions for the multipole moments of $\delta\mathcal{S}^\varepsilon$ and $\delta^2\mathcal{S}^\varepsilon$ in Lemma 4.2.2.

In order to represent the multipole moments (4.22a) and (4.22b) as integral operators in momentum space acting on functions in $\mathcal{D}'(\mathbb{R}^+_0, \mathbb{R})$, however, the remaining momentum space angular integrals have to be carried out. By analogy with the previous subsection, we start by introducing so-called *angular-integrated incomplete Fourier transforms.*

Definition 4.2.6 (Angular-Integrated Incomplete Fourier Transforms)

By slight abuse of notation[a], we define *angular-integrated incomplete Fourier transforms* as

$$\mathcal{F}\big[\mathcal{K}^\varepsilon_{lm}\big](|\vec{p}|) \overset{(4.21a)}{:=} \int_{S^2} \mathrm{d}\Omega_p \; \mathcal{F}\big[\mathcal{K}^\varepsilon_{lm}\big](\vec{p}) \tag{4.30a}$$

$$\begin{Bmatrix} \mathcal{F}\big[\mathcal{M}^\varepsilon_{lm|l'm'}\big](|\vec{p}|,|\vec{q}|) \\ \mathcal{F}\big[\mathcal{N}^\varepsilon_{lm|l'm'}\big](|\vec{p}|,|\vec{q}|) \end{Bmatrix} \overset{(4.21b)}{:=} \int_{S^2} \mathrm{d}\Omega_p \int_{S^2} \mathrm{d}\Omega_q \; \begin{Bmatrix} \mathcal{F}\big[\mathcal{M}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) \\ \mathcal{F}\big[\mathcal{N}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) \end{Bmatrix} \tag{4.30b}$$

$$\begin{Bmatrix} \mathcal{F}\big[\mathcal{V}^\varepsilon_{lm|l'm'}\big](|\vec{p}|,|\vec{q}|) \\ \mathcal{F}\big[\mathcal{W}^\varepsilon_{lm|l'm'}\big](|\vec{p}|,|\vec{q}|) \end{Bmatrix} \overset{(4.21c)}{:=} \int_{S^2} \mathrm{d}\Omega_p \int_{S^2} \mathrm{d}\Omega_q \; \begin{Bmatrix} \mathcal{F}\big[\mathcal{V}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) \\ \mathcal{F}\big[\mathcal{W}^\varepsilon_{lm|l'm'}\big](\vec{p},\vec{q}) \end{Bmatrix} \tag{4.30c}$$

[a]In order to avoid the appearance of another subscript or superscript, we denote the incomplete Fourier transforms and their angular-integrated counterparts by the same symbol $\mathcal{F}[(\bullet)^\varepsilon_{lm|l'm'}]$ and distinguish both only through their arguments $(\vec{p},\vec{q})$ and $(|\vec{p}|,|\vec{q}|)$, respectively.

To compute these angular-integrated incomplete Fourier transforms, we recall that the incomplete Fourier transforms from Lemma 4.2.5 depend on the momentum space angular variables (θ_p, φ_p)

and (θ_q, φ_q) through the (scalar) spherical harmonics $Y_{lm}(\theta_p, \varphi_p)$ and $Y_{l'm'}(\theta_q, \varphi_q)$ and via the arguments $k_\pm := |\vec{p} \pm \vec{q}|$ of the generalized spherical Bessel functions $j_{0,n}(k_\pm r)$. Therefore, the task in this subsection actually boils down to evaluate double integrals of the form

$$\int_{S^2} \mathrm{d}\Omega_p \int_{S^2} \mathrm{d}\Omega_q \; Y_{lm}(\theta_p, \varphi_p) Y_{l'm'}(\theta_q, \varphi_q) j_{0,n}(|\vec{p} \pm \vec{q}|r) \tag{4.31}$$

for arbitrary $n \in \mathbb{Z}$ and $(l,m), (l',m') \in \mathbb{N}_0 \times \mathbb{Z}$ with $-l^{(\prime)} \leq m^{(\prime)} \leq l^{(\prime)}$.

4.2.2.1 The Integral Operators $T_n^\pm$

In order to compute these double integrals in a systematic way, we first introduce the following integral operators.

Definition 4.2.7 (Integral Operator)

Let $\vec{p} \in \mathbb{R}^3$ and $r, |\vec{q}| \in \mathbb{R}_0^+$ be fixed parameters. Then, for any $n \in \mathbb{Z}$, the integral operators $T_n^\pm : L^2(S^2, \mathbb{C}) \to L^2(S^2, \mathbb{C})$ are defined as

$$\big[T_n^\pm(\psi)\big](\hat{\vec{p}}) \overset{(4.26)}{:=} \int_{S^2} \mathrm{d}\Omega_q \; j_{0,n}\big(|\vec{p} \pm \vec{q}|r\big)\psi(\hat{\vec{q}}) \tag{4.32}$$

where the integral kernel is given by the generalized spherical Bessel functions introduced in Definition 4.2.3 and $\hat{\vec{p}} := \vec{p}/|\vec{p}|$ denotes the unit vector in the direction of $\vec{p}$.

To benefit from this definition, we study the properties of this integral operator by first proving its spherical symmetry and then calculating its eigenvalues.

Lemma 4.2.8 (Spherical Symmetry of the Integral Operator $T_n^\pm$)

For any $n \in \mathbb{Z}$, the operators $T_n^\pm$ as introduced in Definition 4.2.7 commute with unitary representations $U_R : L^2(S^2, \mathbb{C}) \to L^2(S^2, \mathbb{C})$ of $R \in \mathrm{SO}(3)$ which act on $\psi \in L^2(S^2, \mathbb{C})$ as

$$\psi(\hat{\vec{p}}) \mapsto \big[U_R(\psi)\big](\hat{\vec{p}}) := \psi(R^{-1}\hat{\vec{p}}) \tag{4.33}$$

where $\hat{\vec{p}} := \vec{p}/|\vec{p}|$ again denotes the unit vector in the direction of $\vec{p}$.

Proof. Let $n \in \mathbb{Z}$ be an arbitrary integer. To show that $T_n^\pm$ commutes with the unitary representation U_R for arbitrary rotations $R \in \mathrm{SO}(3)$, we act with the combined operator $U_R T_n^\pm$ on $\psi \in L^2(S^2, \mathbb{C})$ and use the action of U_R as well as the definition of the integral operator which yields

$$\big[(U_R T_n^\pm)(\psi)\big](\hat{\vec{p}}) = \big[U_R(T_n^\pm \psi)\big](\hat{\vec{p}}) \overset{(4.33)}{=} (T_n^\pm \psi)(R^{-1}\hat{\vec{p}}) \overset{(4.32)}{=} \int_{S^2} \mathrm{d}\Omega_q \; j_{0,n}(|R^{-1}\vec{p} - \vec{q}|r)\psi(\hat{\vec{q}})$$

Rewriting $\vec{q} = R^{-1}(R\vec{q})$, defining the rotated integration variable $\vec{q}_r := R\vec{q}$ and taking into account that rotations do not alter the length of vectors, we find

$$\ldots = \int_{S^2} \mathrm{d}\Omega_q \; j_{0,n}(|R^{-1}(\vec{p} - \vec{q}_r)|r)\psi(R^{-1}\hat{\vec{q}}_r) = \int_{S^2} \mathrm{d}\Omega_{q_r} \; j_{0,n}(|\vec{p} - \vec{q}_r|r)\psi(R^{-1}\hat{\vec{q}}_r)$$

where for the last equality we exploited the fact that the domain of integration as well as the length of vectors are both invariant under rotations. Rewriting $\psi(R^{-1}\hat{\vec{q}}_r) = (U_R\psi)(\hat{\vec{q}}_r)$ and making use of the definition of the integral operator, we finally end up with

$$\ldots \overset{(4.33)}{=} \int_{S^2} \mathrm{d}\Omega_{q_r}\; j_{0,n}(|\vec{p} - \vec{q}_r|r)(U_R\psi)(\hat{\vec{q}}_r) \overset{(4.32)}{=} \big[T^\pm(U_R\psi)\big](\hat{\vec{p}}) = \big[(T^\pm U_R)(\psi)\big](\hat{\vec{p}})$$

This calculation demonstrates that for arbitrary, but fixed parameters $\vec{p} \in \mathbb{R}^3$, $r, |\vec{q}| \in \mathbb{R}_0^+$ and for arbitrary $n \in \mathbb{Z}$, $\psi \in L^2(S^2, \mathbb{C})$ the following relation holds

$$\big[(U_R T^\pm)(\psi)\big](\hat{\vec{p}}) = \big[(T^\pm U_R)(\psi)\big](\hat{\vec{p}}) \qquad \Leftrightarrow \qquad [T^\pm, U_R] = 0 \tag{4.34}$$

which means that for any $n \in \mathbb{Z}$ the integral operators $T_n^\pm : L^2(S^2, \mathbb{C}) \to L^2(S^2, \mathbb{C})$ commute with unitary representations of $R \in \mathrm{SO}(3)$ and are therefore spherically symmetric. □

The spherical symmetry of the integral operators introduced in Definition 4.2.7 greatly simplifies the computation of the eigenvalues.

Lemma 4.2.9 (Eigenfunctions and Eigenvalues of the Integral Operators $T_n^\pm$)

For any $n \in \mathbb{Z}$, the eigenfunctions of the integral operators $T_n^\pm$ as defined in Definition 4.2.7 are spherical harmonics Y_{lm}. For fixed l, the eigenvalue $t_n^\pm(l, m)$ corresponding to the eigenfunction Y_{lm} is independent of m.

Proof. Let $n \in \mathbb{Z}$ be arbitrary but fixed. According to Lemma 4.2.8, the integral operators $T_n^\pm$ as introduced in Definition 4.2.7 commute with unitary representations U_R for arbitrary rotations $R \in \mathrm{SO}(3)$. Due to the fact that the angular momentum operator is the generator of rotations $R \in \mathrm{SO}(3)$, also the integral operators $T_n^\pm$ commute with the angular momentum operator

$$\forall n \in \mathbb{Z}: \qquad \Big[T_n^\pm, \vec{L}\Big] = 0$$

This, in turn, implies via the theorem on eigenfunctions of commuting operators that $T_n^\pm$ and $\vec{L}$ have the same set of eigenfunctions, namely the spherical harmonics Y_{lm}.

Having said this, it remains to determine the eigenvalues $t_n^\pm$ of the operators $T_n^\pm$ and to figure out their dependence on l and m. Supposing that the eigenvalues depend both on l and m[a], we obtain by acting with $T_n^\pm$ on Y_{lm}

$$\forall (l, m) \in \mathbb{N}_0 \times \mathbb{Z} \text{ with } -l \leq m \leq l: \quad t_n^\pm(l, m) Y_{lm}(\hat{\vec{p}}) = T_n^\pm Y_{lm}(\hat{\vec{p}}) \tag{4.35}$$

By exploiting the commutator relation $[T_n^\pm, U_R] \overset{(4.33)}{=} 0$, the operator $T_n^\pm$ on the right-hand side can be rewritten as follows

$$\forall n \in \mathbb{Z}: \quad T_n^\pm = \mathrm{id}\, T_n^\pm = U_R^{-1} U_R T_n^\pm = U_R^{-1} T_n^\pm U_R \tag{4.36}$$

which turns the above equation into

$$t_n^\pm(l, m) Y_{lm}(\hat{\vec{p}}) = U_R^{-1} T_n^\pm U_R Y_{lm}(\hat{\vec{p}}) \overset{(4.33)}{=} U_R^{-1} T_n^\pm Y_{lm}(R^{-1}\hat{\vec{p}}) \tag{4.37}$$

At this point, we choose the so far unspecified rotation $R \in \mathrm{SO}(3)$ such that $R^{-1}\vec{p}$ coincides with the z-axis. As a consequence of this choice we can make use of a special property of spherical harmonics: Evaluating $Y_{lm}(\hat{\vec{p}})$ on the z-axis (i. e. for $\theta_p = 0$), all spherical harmonics except for those with $m = 0$ vanish identically. We thus find

$$t_n^\pm(l,m)Y_{lm}(\hat{\vec{p}}) = U_R^{-1}T_n^\pm Y_{lm}(R^{-1}\hat{\vec{p}}) = U_R^{-1}T_n^\pm Y_{l0}(0,\varphi_p) \overset{(4.35)}{=} U_R^{-1}t_n^\pm(l,0)Y_{l0}(0,\varphi_p) \tag{4.38}$$

Reexpressing $Y_{l0}(0,\varphi_p)$ by $U_R Y_{lm}(\hat{\vec{p}})$ finally results in

$$\forall (l,m) \in \mathbb{N}_0 \times \mathbb{Z} \text{ with } -l \le m \le l: \quad t_n^\pm(l,m)Y_{lm}(\hat{\vec{p}}) = t_n^\pm(l,0)Y_{lm}(\hat{\vec{p}}) \tag{4.39}$$

which demonstrates that for fixed l the eigenvalues are independent of m. This concludes the proof. ☐

[a] As the integral operators $T_n^\pm$ according to Definition 4.2.7 also carry a (not explicitly indicated) dependence on the parameters $r, |\vec{p}|, |\vec{q}| \in \mathbb{R}_0^+$, the eigenvalues may also depend on those parameters. For the sake of clarity, however, we suppress this dependence at this point.

This lemma together with the definition of the integral operators $T_n^\pm$ allows to compute the double integrals in (4.31) as follows.

Proposition 4.2.10 (Evaluation of Momentum Space Angular Integrals)

The momentum space angular integrals appearing in the angular-integrated incomplete Fourier transforms evaluate to

$$\int_{S^2} \mathrm{d}\Omega_p\ Y_{lm}(\theta_p,\varphi_p) j_{0,1}(|\vec{p}|r) = \frac{\delta_{l0}\delta_{m0}}{\sqrt{4\pi}} t_1^\pm(0,r,|\vec{p}|,0) \tag{4.40a}$$

$$\int_{S^2} \mathrm{d}\Omega_p \int_{S^2} \mathrm{d}\Omega_q\ Y_{lm}(\theta_p,\varphi_p) Y_{l'm'}(\theta_q,\varphi_q) j_{0,n}(|\vec{p}\pm\vec{q}|r) = t_n^\pm(l',r,|\vec{p}|,|\vec{q}|)\times \\ \times (-1)^{m'}\delta_{ll'}\delta_{m(-m')} \tag{4.40b}$$

where $t_n^\pm(l',r,|\vec{p}|,|\vec{q}|)$ denote the eigenvalues of the integral operators introduced in Definition 4.2.7.

Proof. For the angular-integrated incomplete Fourier transform of $\mathcal{F}\big[\mathcal{K}_{lm}^\varepsilon\big](\vec{p})$ we have to evaluate only one momentum space angular integral. Carrying out this integral by using the orthogonality properties of the spherical harmonics yields

$$\int_{S^2} \mathrm{d}\Omega_p\ Y_{lm}(\theta_p,\varphi_p) j_{0,1}(|\vec{p}|r) = \\ \sqrt{4\pi} j_{0,1}(|\vec{p}|r) \int_{S^2} \mathrm{d}\Omega_p\ Y_{lm}(\theta_p,\varphi_p) Y_{00}(\theta_p,\varphi_p) = \frac{\delta_{l0}\delta_{m0}}{\sqrt{4\pi}} t_1^\pm(0,r,|\vec{p}|,0) \tag{4.41}$$

Note that for the second equality we used the fact that the generalized spherical Bessel function $j_{0,1}(|\vec{p}|r)$ is related to the eigenvalues $t_n^\pm$ via $4\pi j_{0,1}(|\vec{p}|r) = t_1^\pm(0,r,|\vec{p}|,0)$ which can be derived in anticipation of Lemma 4.2.13.

For all other angular-integrated incomplete Fourier transforms there are two momentum space angular integrals. Expressing them in terms of the integral operators $T_n^\pm$ and making use of Lemma 4.2.9 yields

$$\int_{S^2} \mathrm{d}\Omega_p \int_{S^2} \mathrm{d}\Omega_q\ Y_{lm}(\theta_p,\varphi_p) Y_{l'm'}(\theta_q,\varphi_q) j_{0,n}(|\vec{p}\pm\vec{q}|r) =$$

$$\overset{(4.32)}{=} \int\limits_{S^2} \mathrm{d}\Omega_p \; Y_{lm}(\theta_p,\varphi_p) T_n^{\pm} Y_{l'm'}(\theta_p,\varphi_p)$$
$$= t_n^{\pm}(l',r,|\vec{p}|,|\vec{q}|) \int\limits_{S^2} \mathrm{d}\Omega_p \; Y_{lm}(\theta_p,\varphi_p) Y_{l'm'}(\theta_p,\varphi_p)$$
$$= t_n^{\pm}(l',r,|\vec{p}|,|\vec{q}|)(-1)^{m'} \delta_{ll'}\delta_{m(-m')} \tag{4.42}$$

where in the last step we again exploited the orthogonality relations for spherical harmonics. □

Before we proceed, we recall that the matrix-valued differential operators $\mathfrak{m}^{(n)}$, $\mathfrak{n}^{(n)}$ and $\overset{*}{\mathfrak{m}}^{(n)}$, $\overset{*}{\mathfrak{n}}^{(n)}$ act on the generalized spherical Bessel functions $j_{0,n}(k_\pm r)$. Combining this fact with the result from Proposition 4.2.10 suggests to introduce the following matrix-valued functions.

Definition 4.2.11 (Multipole Matrices)

For $l,l' \in \mathbb{N}_0$, the matrix-valued functions $\mathfrak{K}_0 : (\mathbb{R}_0^+)^2 \to \mathbb{R}^{5\times5}$ and $\mathfrak{M}_{ll'}, \mathfrak{N}_{ll'}, \overset{*}{\mathfrak{M}}_{ll'}, \overset{*}{\mathfrak{N}}_{ll'} : (\mathbb{R}_0^+)^3 \to \mathbb{R}^{5\times5}$, referred to as *multipole matrices*, are defined as

$$\mathfrak{K}_0(r,|\vec{p}|) := \mathfrak{k}^{(1)}(r,|\vec{p}|) t_1^{\pm}(0,r,|\vec{p}|,0) \tag{4.43a}$$

$$\overset{(*)}{\mathfrak{M}}_{ll'}(r,|\vec{p}|,|\vec{q}|) := \sum_{\substack{n=-1 \\ n \text{ odd}}}^{5} \overset{(*)}{\mathfrak{m}}^{(n)}(l,l',r,|\vec{p}|,|\vec{q}|) t_n^{+}(l',r,|\vec{p}|,|\vec{q}|) \tag{4.43b}$$

$$\overset{(*)}{\mathfrak{N}}_{ll'}(r,|\vec{p}|,|\vec{q}|) := \sum_{\substack{n=-1 \\ n \text{ odd}}}^{5} \overset{(*)}{\mathfrak{n}}^{(n)}(l,l',r,|\vec{p}|,|\vec{q}|) t_n^{-}(l',r,|\vec{p}|,|\vec{q}|) \tag{4.43c}$$

where $\mathfrak{k}^{(1)}$ and $\mathfrak{m}^{(n)}$, $\mathfrak{n}^{(n)}$ as well as their asterisked counterparts denote the matrix-valued derivative operators with respect to r as defined in Definition C.4.2.

These matrix-valued functions, in turn, allow to express the angular integrated incomplete Fourier transforms introduced in Definition 4.2.6 as follows.

Lemma 4.2.12 (Angular-Integrated Incomplete Fourier Transforms)

The non-vanishing angular-integrated incomplete Fourier transforms evaluate to

$$\mathcal{F}\big[\mathcal{K}_{00}^\varepsilon\big](|\vec{p}|) = \int\limits_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0,r) \; \frac{r^2 E_{\mathcal{K}}^\varepsilon}{\sqrt{4\pi}} \big(\mathcal{C}_{\mathcal{K}}^\varepsilon \odot \mathfrak{K}_0\big) \tag{4.44a}$$

$$\begin{Bmatrix} \mathcal{F}\big[\mathcal{M}_{lm|l(-m)}^\varepsilon\big](|\vec{p}|,|\vec{q}|) \\ \mathcal{F}\big[\mathcal{N}_{lm|l(-m)}^\varepsilon\big](|\vec{p}|,|\vec{q}|) \end{Bmatrix} = \int\limits_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0,r) \begin{Bmatrix} (-1)^{-m} r^2 E_{\mathcal{M}}^\varepsilon \big(\mathcal{C}_{\mathcal{M}}^\varepsilon \odot \mathfrak{M}_{ll} + C^\varepsilon \overset{*}{\mathfrak{M}}_{ll}\big) \\ r^2 E_{\mathcal{N}}^\varepsilon \big(\mathcal{C}_{\mathcal{N}}^\varepsilon \odot \mathfrak{N}_{ll} - B^\varepsilon \overset{*}{\mathfrak{N}}_{ll}\big) \end{Bmatrix} \tag{4.44b}$$

$$\begin{Bmatrix} \mathcal{F}\big[\mathcal{V}_{lm|l(-m)}^\varepsilon\big](|\vec{p}|,|\vec{q}|) \\ \mathcal{F}\big[\mathcal{W}_{lm|l(-m)}^\varepsilon\big](|\vec{p}|,|\vec{q}|) \end{Bmatrix} = \int\limits_{\mathbb{R}} \mathrm{d}\xi^0 \left.\begin{Bmatrix} (-1)^{-m} r^2 E_{\mathcal{V}}^\varepsilon \big(\mathcal{C}_{\mathcal{V}}^\varepsilon \odot \mathfrak{M}_{ll}\big) \\ r^2 E_{\mathcal{W}}^\varepsilon \big(\mathcal{C}_{\mathcal{W}}^\varepsilon \odot \mathfrak{N}_{ll}\big) \end{Bmatrix}\right|_{r=R_{\max}^\varepsilon(\xi^0)} \tag{4.44c}$$

where $\mathcal{C}_\bullet^\varepsilon$ denote the coefficient matrices (see (4.13a), (4.19a,i), (4.19b,i), (4.24a,ii), (4.24b,ii)), $E_\bullet^\varepsilon$ the corresponding functions containing the exponential factor as well as the regularization of the mass shell (see (4.13b), (4.19a,ii), (4.19b,ii), (4.24a,i), (4.24b,i)) and $\mathfrak{K}_0$, $\mathfrak{M}_{ll}$, $\mathfrak{N}_{ll}$ as well as their asterisked counterparts are the multipole matrices from Definition 4.2.11.

Proof. To arrive at the claimed expressions, we insert the incomplete Fourier transforms from Lemma 4.2.5 into Definition 4.2.6 and subsequently carry out the angular integrals using the results from Proposition 4.2.10. Note that as a consequence of the orthogonality relations of the spherical harmonics, only those angular-integrated incomplete Fourier transforms with $l = l'$ and $m = -m'$ are non-vanishing. Finally, by expressing everything in terms of the multipole matrices we end up with the claimed expressions. This concludes the proof. □

We emphasize that these angular-integrated incomplete Fourier transforms contain the full information about the chosen regularization of the unperturbed, spherically-symmetrically regularized kernel of the fermionic projector (via the functions $R^{\varepsilon}_{\max}$ and $E^{\varepsilon}_{\bullet}$ as well as the coefficient matrices $\mathfrak{C}^{\varepsilon}_{\bullet}$) and additionally provide information about the weight of the contribution depending on the multipole order l.

4.2.2.2 Closed-Form Expression for the Eigenvalues of $T_n^{\pm}$

In Lemma 4.2.9 we have shown that the eigenvalues $t_n^{\pm}$ of the integral operators $T_n^{\pm}$ depend on the multipole order l, but not on the parameter m. In order to quantify this dependence on l as well as the dependence on the other variables r, $|\vec{p}|$ and $|\vec{q}|$, it remains to work out an explicit expression for the eigenvalues contained in the multipole matrices $\mathfrak{M}_{ll}$, $\mathfrak{N}_{ll}$ and $\overset{*}{\mathfrak{M}}_{ll}$, $\overset{*}{\mathfrak{N}}_{ll}$.

Lemma 4.2.13 (Computation of the Eigenvalues of the Integral Operators $T_n^{\pm}$)

The eigenvalues $t_n^{\pm}(l, r, |\vec{p}|, |\vec{q}|)$ of the integral operators $T_n^{\pm}$ as introduced in Definition 4.2.7 are given by

$$t_n^{\pm}(l, r, |\vec{p}|, |\vec{q}|) = \left(\mp \frac{(|\vec{p}| \mp |\vec{q}|)^2}{4|\vec{p}||\vec{q}|} \right)^l \sum_{k=0}^{l} \left[\binom{l}{k} \right]^2 \left(\frac{|\vec{p}| \pm |\vec{q}|}{|\vec{p}| \mp |\vec{q}|} \right)^{2k} \sum_{i=0}^{k} \binom{k}{i} \sum_{j=0}^{l-k} \binom{l-k}{j} \times$$
$$\times \left(\frac{-1}{(|\vec{p}| \pm |\vec{q}|)^2} \right)^i \left(\frac{-1}{(|\vec{p}| \mp |\vec{q}|)^2} \right)^j \frac{2\pi I^{\pm}_{n-2(i+j)}(r\sigma, \rho)}{r^n \sigma^{n-2(i+j)}} \tag{4.45}$$

where the functions $I^{\pm}_{n-2(i+j)}$ are those introduced in Definition D.1.1 and the parameters ρ, σ are defined as

$$\rho := \frac{2|\vec{p}||\vec{q}|}{|\vec{p}|^2 + |\vec{q}|^2} \qquad \text{and} \qquad \sigma := \sqrt{|\vec{p}|^2 + |\vec{q}|^2} \tag{4.45a}$$

At multipole orders $l = 0$ and $l = 1$ the eigenvalues reduce to

$$t_n^{\pm}(0, r, |\vec{p}|, |\vec{q}|) = \frac{2\pi}{(r\sigma)^n} I_n^{\pm}(r\sigma, \rho) \tag{4.46a}$$

$$t_n^{\pm}(1, r, |\vec{p}|, |\vec{q}|) = \mp \frac{2\pi}{(r\sigma)^n} \frac{1}{\rho} \Big[I_n^{\pm}(r\sigma, \rho) - I^{\pm}_{n-2}(r\sigma, \rho) \Big] \tag{4.46b}$$

Proof. In order to compute the eigenvalues $t_n^{\pm}(l, r, |\vec{p}|, |\vec{q}|)$, we make use of Lemma 4.2.9 according to which the eigenvalues are independent of m for fixed l. Thus, without loss of generality, we can choose to act with $T_n^{\pm}$ on $Y_{l0}(\theta_p, \varphi_p) \equiv Y_{l0}(\hat{\vec{p}})$ which yields

$$t_n^{\pm}(l, r, |\vec{p}|, |\vec{q}|) Y_{l0}(\hat{\vec{p}}) = T_n^{\pm} Y_{l0}(\hat{\vec{p}}) \tag{4.47}$$

Acting on this equation with U_R for an arbitrary rotation $R \in \mathrm{SO}(3)$, exploiting the spherical symmetry (which, according to Lemma 4.2.8, allows to replace $U_R T_n^{\pm}$ by $T_n^{\pm} U_R$) on the right-hand side and dividing by $U_R Y_{l0}(\hat{\vec{p}})$ results in

$$t_n^{\pm}(l, r, |\vec{p}|, |\vec{q}|) = \frac{T_n^{\pm} U_R Y_{l0}(\hat{\vec{p}})}{U_R Y_{l0}(\hat{\vec{p}})} \tag{4.48}$$

By choosing the rotation $R \in \mathrm{SO}(3)$ such that the vector $R^{-1}\vec{p}$ coincides with the z-axis in the new, rotated coordinate system (we take the viewpoint of a *passive* transformation), we obtain

$$t_n^{\pm}(l, r, |\vec{p}|, |\vec{q}|) = \frac{T_n^{\pm} Y_{l0}(R^{-1}\hat{\vec{p}})}{Y_{l0}(R^{-1}\hat{\vec{p}})} \overset{(4.32)}{=} \frac{1}{Y_{l0}(R^{-1}\hat{\vec{p}})} \int_{S^2} \mathrm{d}\Omega_q \; j_{0,n}(|R^{-1}\vec{p} \pm \vec{q}|r) Y_{l0}(\hat{\vec{q}}) \tag{4.49}$$

To proceed, we need the explicit form of $Y_{l0}(\hat{\vec{q}})$ which according to Definition 4.1.3 is given by

$$Y_{l0}(\hat{\vec{q}}) \overset{(4.5a)}{=} \sqrt{\frac{2l+1}{4\pi}} \frac{1}{2^l l!} \frac{\mathrm{d}^l (x^2-1)^l}{\mathrm{d}x^l} \bigg|_{x=\cos(\theta_q)}$$

Carrying out the l-fold derivative by factorizing $(x^2-1)^l = (x-1)^l (x+1)^l$ and using the general Leibniz rule turns the expression into

$$Y_{l0}(\hat{\vec{q}}) = \sqrt{\frac{2l+1}{4\pi}} \frac{1}{2^l l!} \sum_{k=0}^{l} \binom{l}{k} \frac{(l!)^2}{(l-k)!k!} (\cos(\theta_q) - 1)^k (\cos(\theta_q) + 1)^{l-k}$$

Furthermore, as a consequence of the specific choice of the rotation $R \in \mathrm{SO}(3)$ such that $R^{-1}\vec{p}$ coincides with the z-axis, we have

$$|R^{-1}\vec{p} \pm \vec{q}|^2 = |R^{-1}\vec{p}|^2 + |\vec{q}|^2 \pm 2|R^{-1}\vec{p}||\vec{q}|\cos(\theta_q) = |\vec{p}|^2 + |\vec{q}|^2 \pm 2|\vec{p}||\vec{q}|\cos(\theta_q)$$

where we used the fact that rotations do not change lengths of vectors. Inserting the expression for $Y_{l0}(\hat{\vec{q}})$ into the formula for $t_n^{\pm}(l, r, |\vec{p}|, |\vec{q}|)$ and replacing all occurrences of $\cos(\theta_q)$ according to the above relation in terms of $|R^{-1}\vec{p} \pm \vec{q}|^2$ leads to

$$\begin{aligned}
t_n^{\pm}(l, r, |\vec{p}|, |\vec{q}|) &= \frac{\sqrt{\frac{2l+1}{4\pi}}}{Y_{l0}(R^{-1}\hat{\vec{p}})} \frac{1}{2^l l!} \sum_{k=0}^{l} \binom{l}{k} \frac{(l!)^2}{(l-k)!k!} \int_{S^2} \mathrm{d}\Omega_q \; j_{0,n}(|R^{-1}\vec{p} \pm \vec{q}|r) \times \\
&\quad \times \left(\pm \frac{|R^{-1}\vec{p} \pm \vec{q}|^2 - |\vec{p}|^2 - |\vec{q}|^2}{2|\vec{p}||\vec{q}|} - 1 \right)^k \left(\pm \frac{|R^{-1}\vec{p} \pm \vec{q}|^2 - |\vec{p}|^2 - |\vec{q}|^2}{2|\vec{p}||\vec{q}|} + 1 \right)^{l-k} \\
&= \frac{\sqrt{\frac{2l+1}{4\pi}}}{Y_{l0}(R^{-1}\hat{\vec{p}})} \left(\frac{1}{4|\vec{p}||\vec{q}|} \right)^l \sum_{k=0}^{l} \left[\binom{l}{k} \right]^2 \int_{S^2} \mathrm{d}\Omega_q \; j_{0,n}(|R^{-1}\vec{p} \pm \vec{q}|r) \times \\
&\quad \times \big(\pm |R^{-1}\vec{p} \pm \vec{q}|^2 \mp (|\vec{p}| \pm |\vec{q}|)^2 \big)^k \big(\pm |R^{-1}\vec{p} \pm \vec{q}|^2 \mp (|\vec{p}| \mp |\vec{q}|)^2 \big)^{l-k}
\end{aligned}$$

Rewriting the two factors in the second line each using the binomial theorem gives

$$\begin{aligned}
\ldots = \frac{\sqrt{\frac{2l+1}{4\pi}}}{Y_{l0}(R^{-1}\hat{\vec{p}})} \left(\frac{\mp 1}{4|\vec{p}||\vec{q}|} \right)^l \sum_{k=0}^{l} \left[\binom{l}{k} \right]^2 (|\vec{p}| \pm |\vec{q}|)^{2k} (|\vec{p}| \mp |\vec{q}|)^{2(l-k)} \times \\
\times \sum_{i=0}^{k} \binom{k}{i} \sum_{j=0}^{l-k} \binom{l-k}{j} \left(\frac{-1}{(|\vec{p}| \pm |\vec{q}|)^2} \right)^i \left(\frac{-1}{(|\vec{p}| \mp |\vec{q}|)^2} \right)^j \times \\
\times \int_{S^2} \mathrm{d}\Omega_q \; j_{0,n}(|R^{-1}\vec{p} \pm \vec{q}|r) \big(|R^{-1}\vec{p} \pm \vec{q}|^2 \big)^{i+j}
\end{aligned}$$

Taking into account that according to our choice of the rotation the factor $Y_{l0}(R^{-1}\hat{\vec{p}})$ evaluates to $Y_{l0}(R^{-1}\hat{\vec{p}}) = Y_{l0}(0, \varphi) = \sqrt{\frac{2l+1}{4\pi}}$ and that in the remaining integral $|R^{-1}\vec{p} \pm \vec{q}|^2$ can be replaced by $|\vec{p}|^2 + |\vec{q}|^2 \pm 2|\vec{p}||\vec{q}|\cos(\theta_q)$, we find the following expression for the eigenvalues

$$t_n^{\pm}(l, r, |\vec{p}|, |\vec{q}|) = \left(\mp \frac{(|\vec{p}| \mp |\vec{q}|)^2}{4|\vec{p}||\vec{q}|} \right)^l \sum_{k=0}^{l} \left[\binom{l}{k} \right]^2 \left(\frac{|\vec{p}| \pm |\vec{q}|}{|\vec{p}| \mp |\vec{q}|} \right)^{2k} \times$$

$$\times \sum_{i=0}^{k} \binom{k}{i} \sum_{j=0}^{l-k} \binom{l-k}{j} \left(\frac{-1}{(|\vec{p}| \pm |\vec{q}|)^2} \right)^i \left(\frac{-1}{(|\vec{p}| \mp |\vec{q}|)^2} \right)^j \times$$
$$\times \frac{1}{r^n} \int_{-1}^{1} \mathrm{d}\cos(\theta_q) \int_{0}^{2\pi} \mathrm{d}\varphi_q \, \frac{\sin\left(r\sqrt{|\vec{p}|^2 + |\vec{q}|^2 \pm 2|\vec{p}||\vec{q}|\cos(\theta_q)}\right)}{\sqrt{|\vec{p}|^2 + |\vec{q}|^2 \pm 2|\vec{p}||\vec{q}|\cos(\theta_q)}^{\,n-2(i+j)}}$$

By carrying out the azimuthal integral and defining parameters

$$\rho := \frac{2|\vec{p}||\vec{q}|}{|\vec{p}|^2 + |\vec{q}|^2} \qquad \text{and} \qquad \sigma := \sqrt{|\vec{p}|^2 + |\vec{q}|^2}$$

the remaining integral can be expressed in terms of the functions $I_n^{\pm}$ introduced in Definition D.1.1 where we identify $\alpha = r\sigma$ such that we finally end up with

$$t_n^{\pm}(l, r, |\vec{p}|, |\vec{q}|) = \left(\mp \frac{(|\vec{p}| \mp |\vec{q}|)^2}{4|\vec{p}||\vec{q}|} \right)^l \sum_{k=0}^{l} \left[\binom{l}{k} \right]^2 \left(\frac{|\vec{p}| \pm |\vec{q}|}{|\vec{p}| \mp |\vec{q}|} \right)^{2k} \sum_{i=0}^{k} \binom{k}{i} \sum_{j=0}^{l-k} \binom{l-k}{j} \times$$
$$\times \left(\frac{-1}{(|\vec{p}| \pm |\vec{q}|)^2} \right)^i \left(\frac{-1}{(|\vec{p}| \mp |\vec{q}|)^2} \right)^j \frac{2\pi I^{\pm}_{n-2(i+j)}(r\sigma, \rho)}{r^n \sigma^{n-2(i+j)}} \tag{4.50}$$

This concludes the proof. □

This lemma now allows us to evaluate the multipole matrices introduced in Definition 4.2.11. The resulting explicit expressions for $\mathfrak{K}_0$, $\mathfrak{M}_{ll}$, $\mathfrak{N}_{ll}$ and their asterisked counterparts $\overset{*}{\mathfrak{M}}_{ll}$, $\overset{*}{\mathfrak{N}}_{ll}$ at the two lowest multipole orders $l = 0$ and $l = 1$ can be found in Appendix E.

4.3 Summary: Integral Operators for $\delta\mathcal{S}_l^{\varepsilon}$ and $\delta^2\mathcal{S}_l^{\varepsilon}$

Having derived a closed-form expression for the eigenvalues, we can evaluate the angular-integrated incomplete Fourier transforms for arbitrary $(l, m) \in \mathbb{N}_0 \times \mathbb{Z}$ with $-l \leq m \leq l$. Putting together all the above results, the multipole expansions of $\delta\mathcal{S}^{\varepsilon}$ and $\delta^2\mathcal{S}^{\varepsilon}$ from Lemma 4.2.2 can be expressed in terms of integral operators with matrix-valued integral kernels.

Theorem 4.3.1 (Multipole Expansion of $\delta\mathcal{S}^{\varepsilon}$ and $\delta^2\mathcal{S}^{\varepsilon}$)

Let $\delta\mathcal{S}^{\varepsilon}$ and $\delta^2\mathcal{S}^{\varepsilon}$ be the variations of the regularized causal action as derived in Theorem 3.4.3. The non-vanishing multipole moments in the multipole expansions

$$\delta\mathcal{S}^{\varepsilon} = \sum_{l=0}^{\infty} \delta\mathcal{S}_l^{\varepsilon} \qquad \text{and} \qquad \delta^2\mathcal{S}^{\varepsilon} = \sum_{l=0}^{\infty} \delta^2\mathcal{S}_l^{\varepsilon} \tag{4.51}$$

are given by

$$\delta\mathcal{S}_0^{\varepsilon} = \mathrm{Re}\left[\left\langle\!\!\left\langle \mathbb{1}_{5\times 1}, \mathrm{R}_{00}^{\varepsilon} \Delta_{00} \right\rangle\!\!\right\rangle \right] \tag{4.51a}$$

$$\delta^2\mathcal{S}_l^{\varepsilon} = \mathrm{Re}\left[\delta_{l0} \cdot \left\langle\!\!\left\langle \mathbb{1}_{5\times 1}, \mathrm{R}_{00}^{\varepsilon} (\Delta^2)_{00} \right\rangle\!\!\right\rangle + \frac{1}{2} \sum_{m=-l}^{l} \left\langle\!\!\left\langle \Delta_{lm}, \mathrm{S}_{lm}^{\varepsilon} \Delta_{lm} \right\rangle\!\!\right\rangle \right] \tag{4.51b}$$

where $(\Delta^{(n)})_{lm} \in \mathcal{D}'(\mathbb{R}_0^+, \mathbb{C}^5)$ denotes the vector of multipole moments of the variations of the regularized kernel of the fermionic projector and where $\langle\!\langle \cdot, \cdot \rangle\!\rangle : C^{\infty}(\mathbb{R}_0^+, \mathbb{C}^5) \times C^{\infty}(\mathbb{R}_0^+, \mathbb{C}^5) \to \mathbb{C}$

is the sesquilinear form given by

$$(f,g) \mapsto \langle\!\langle f,g \rangle\!\rangle := \int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4} \sum_{k=1}^{5} f_k(|\vec{p}|)\overline{g_k(|\vec{p}|)} \tag{4.52}$$

Furthermore, the multiplication operator $\mathrm{R}_{00}^\varepsilon : C^\infty(\mathbb{R}_0^+, \mathbb{C}^5) \to C^\infty(\mathbb{R}_0^+, \mathbb{C}^5)$ as well as the integral operators $\mathrm{S}_{lm}^\varepsilon : C^\infty(\mathbb{R}_0^+, \mathbb{C}^5) \to C^\infty(\mathbb{R}_0^+, \mathbb{C}^5)$ for $(l,m) \in \mathbb{N}_0 \times \mathbb{Z}$ with $-l \le m \le l$, which are defined in terms of the angular-integrated incomplete Fourier transforms, read

$$\big(\mathrm{R}_{00}^\varepsilon \Delta_{lm}\big)(|\vec{p}|) := \overline{\mathcal{F}\big[\mathcal{K}_{00}^\varepsilon\big](|\vec{p}|)}\Delta_{lm}(|\vec{p}|) \tag{4.53a}$$

$$\begin{aligned}\big(\mathrm{S}_{lm}^\varepsilon \Delta_{lm}\big)(|\vec{p}|) := \int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4} \Big[&\overline{\mathcal{F}\big[\mathcal{N}_{lm|l(-m)}^\varepsilon\big](|\vec{p}|,|\vec{q}|)} - \overline{\mathcal{F}\big[\mathcal{W}_{lm|l(-m)}^\varepsilon\big](|\vec{p}|,|\vec{q}|)} \\ &+ (-1)^{-m}\overline{\mathcal{F}\big[\mathcal{M}_{lm|l(-m)}^\varepsilon\big](|\vec{p}|,|\vec{q}|)} \\ &- (-1)^{-m}\overline{\mathcal{F}\big[\mathcal{V}_{lm|l(-m)}^\varepsilon\big](|\vec{p}|,|\vec{q}|)}\Big]\Delta_{lm}(|\vec{q}|)\end{aligned} \tag{4.53b}$$

Proof. In order to arrive at the claimed expressions, we basically have to combine all the results from the previous sections in the right way. To describe this procedure in some detail, though without being too repetitive, we sketch the main steps using the example of one of the terms in the sesquilinear contribution to the second variation.[a]

(1) Starting Point: Multipole Moment $\delta^2\mathcal{S}_{lm|l'm'}^\varepsilon$ from Lemma 4.2.2

We start from the expressions for the multipole moments of $\delta\mathcal{S}^\varepsilon$ and $\delta^2\mathcal{S}^\varepsilon$ as given in (4.22a) and (4.22b). The latter, with respect to its structure, has the following schematic form

$$\begin{aligned}\delta^2\mathcal{S}_{lm|l'm'}^\varepsilon \overset{(4.22b)}{=} \mathrm{Re}\Bigg\{ &\int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}}{(2\pi)^4} \begin{pmatrix}\text{linear contribution} \\ \text{in } (\Delta^2)_{lm}^\varepsilon(|\vec{p}|)\end{pmatrix} + \frac{1}{2}\int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}}{(2\pi)^4}\int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{q}}{(2\pi)^4} \times \\ &\times \Delta_{lm}^\varepsilon(|\vec{p}|)^{\mathrm{T}}\left[(-1)^{m'}\mathcal{F}\big[\mathcal{M}_{lm|l'm'}^\varepsilon\big](\vec{p},\vec{q}) + \begin{pmatrix}\text{further terms in the} \\ \text{sesquilinear contrib.}\end{pmatrix}\right]\overline{\Delta_{l'(-m')}^\varepsilon(|\vec{q}|)}\Bigg\}\end{aligned}$$

Here the dependence on the scalar and vector spherical harmonics is encoded in the incomplete Fourier transforms which, again illustrated by the example of $\mathcal{F}\big[\mathcal{M}_{lm|l'm'}^\varepsilon\big]$, are given by

$$\mathcal{F}\big[\mathcal{M}_{lm|l'm'}^\varepsilon\big](\vec{p},\vec{q}) \overset{(4.21b)}{=} \int_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0,r) \int_{S^2} \mathrm{d}\Omega_\xi\ r^2\big(\mathcal{C}_\mathcal{M}^\varepsilon \odot \Upsilon_{lm|l'm'} + C^\varepsilon \overset{*}{\Upsilon}_{lm|l'm'}\big)E_\mathcal{M}^\varepsilon \mathrm{e}^{-\mathrm{i}(\vec{p}+\vec{q})\cdot\vec{\xi}}$$

(2) Simplification, Part 1: Position Space Angular Integration

To distill the effective dependence of $\delta^2\mathcal{S}_{lm|l'm'}^\varepsilon$ on the multipole order l, we first eliminate the position space angular variables by carrying out the corresponding integrals using Lemma 4.2.5 as described in Subsection 4.2.1. This, again focusing only on the term $\mathcal{F}\big[\mathcal{M}_{lm|l'm'}^\varepsilon\big]$, results in

$$\mathcal{F}\big[\mathcal{M}_{lm|l'm'}^\varepsilon\big](\vec{p},\vec{q}) \overset{(4.29b)}{=} \sum_{\substack{n=-1 \\ n \text{ odd}}}^{5} \int_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0,r)\ r^2 Y_{lm}Y_{l'm'}E_\mathcal{M}^\varepsilon\big(\mathcal{C}_\mathcal{M}^\varepsilon \odot \mathfrak{m}^{(n)} + C^\varepsilon \overset{*}{\mathfrak{m}}^{(n)}\big)j_{0,n}(k_+ r)$$

The matrices $\Upsilon_{lm|l'm'}$ and $\overset{*}{\Upsilon}_{lm|l'm'}$ of spherical harmonics have turned into a product of *scalar* spherical harmonics $Y_{lm}Y_{l'm'}$ and a sum of matrix-valued differential operators $\mathfrak{m}^{(n)}$ and $\overset{*}{\mathfrak{m}}^{(n)}$ acting on the generalized spherical Bessel functions $j_{0,n}(k_\pm(\vec{p},\vec{q})r)$, while the coefficient matrix $\mathcal{C}_\mathcal{M}^\varepsilon$ remains unchanged.[b]

(3) Simplification, Part 2: Momentum Space Angular Integration
Next one can eliminate the momentum space angular variables by using the central result from Subsection 4.2.2, namely Lemma 4.2.12. The angular-integrated incomplete Fourier transforms $\mathcal{F}\big[\mathcal{M}^\varepsilon_{lm|l'm'}\big](|\vec{p}|,|\vec{q}|)$ are non-vanishing only for $(l',m')=(l,-m)$ and read

$$\mathcal{F}\big[\mathcal{M}^\varepsilon_{lm|l(-m)}\big](|\vec{p}|,|\vec{q}|) \overset{(4.44b)}{=} \int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0,r)\ (-1)^{-m} r^2 E^\varepsilon_{\mathcal{M}}\big(\mathfrak{C}^\varepsilon_{\mathcal{M}} \odot \mathfrak{M}_{ll} + C^\varepsilon \overset{*}{\mathfrak{M}}_{ll}\big)$$

In this way, the multipole moments $\delta^2\mathcal{S}^\varepsilon_{lm|l'm'}$ reduce to

$$\begin{aligned}\delta^2\mathcal{S}^\varepsilon_{lm|l(-m)} \overset{(4.22b)}{=} \mathrm{Re}\Bigg\{ &\int_{\mathbb{R}^3} \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4} \begin{pmatrix}\text{linear contribution}\\ \text{in } (\Delta^2)^\varepsilon_{lm}(|\vec{p}|)\end{pmatrix} + \frac{1}{2}\int_{\mathbb{R}^3} \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4} \int_{\mathbb{R}^3} \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\ \times \\ &\times \Delta^\varepsilon_{lm}(|\vec{p}|)^{\mathrm{T}} \left[(-1)^{-m}\mathcal{F}\big[\mathcal{M}^\varepsilon_{lm|l'm'}\big](|\vec{p}|,|\vec{q}|) + \begin{pmatrix}\text{further terms in the}\\ \text{sesquilinear contrib.}\end{pmatrix}\right] \overline{\Delta^\varepsilon_{lm}(|\vec{q}|)}\Bigg\}\end{aligned}$$

(4) Definition of Sesquilinear Form and Integral Operators
Having arrived at this point it remains to rewrite the above expression by introducing the sesquilinear form (4.52) along with operators $\mathrm{R}^\varepsilon_{00}, \mathrm{S}^\varepsilon_{lm} : C^\infty(\mathbb{R}^+_0, \mathbb{C}^5) \to C^\infty(\mathbb{R}^+_0, \mathbb{C}^5)$ as in (4.53). Finally, by pulling the sum over m inside, we end up with the claimed expressions for the multipole moments.

This concludes the proof. □

[a] Note that for all other terms in the sesquilinear contribution to the second variation the procedure is exactly the same; for the linear contribution and the whole first variation (which, after replacing Δ^2 by Δ is the same as the linear contribution to the second variation) a simplified version of the procedure applies.

[b] For the linear term and the first variation, the dependence on the angular variables (θ_p,φ_p) only enters through the spherical harmonics $Y_{lm}(\theta_p,\varphi_p)$ which, in the next step, makes the angular momentum integration in momentum space rather easy.

Part III

Applications

Special Perturbations, Variations of the Local Particle Density and Invertibility of $\delta^2\mathcal{S}^\varepsilon$

5

Special Perturbations, Compensations and Variations of the Local Particle Density

Contents

In this chapter we take the multipole expansions of the variations of the regularized causal action as derived in Theorem 4.3.1 for a certain class or regularized kernels of the fermionic projector as our starting point and apply it to concrete problems where a specific regularization is given.

In Section 5.1 we start by customizing the expressions for the non-vanishing multipole moments $\delta\mathcal{S}_0^{\varepsilon}$ and $\delta^2\mathcal{S}_{lm}^{\varepsilon}$ as given in (4.51a) and (4.51b), respectively, to the case where the regularization of the kernel of the fermionic projector is given by an anisotropic version of the ordinary iε-regularization. By deriving explicit expressions for the variation of the regularized kernel of the fermionic projector corresponding to Lorentz boosts, we show in Section 5.2 that the expressions for $\delta\mathcal{S}^{\varepsilon}$ and $\delta^2\mathcal{S}^{\varepsilon}$ as derived in Theorem 5.1.4 vanish and thus demonstrate that the iε-regularized causal action is invariant under Lorentz boosts.

Afterwards, again building on the result from Theorem 5.1.4, we come back to general anisotropically deformed iε-regularized kernels of the fermionic projector and study how variations of the regularized causal action can be balanced by so-called *compensations*. Finally, in Subsection 5.3.2 we derive an expression for the variation of the local particle density of the iε-regularized Dirac sea configuration and show that it is vanishing at first order, but non-vanishing at second order even for Lorentz boosts. This fact, in combination with the results from Theorem 5.2.5 and Theorem 6.3.3 motivates a novel mechanism of baryogenesis within the framework of causal fermion systems.[77]

5.1 Anisotropic Perturbations of iε-Regularized $\widehat{\mathrm{P}^\varepsilon}$

The underlying assumption of the whole chapter is that the so-far unspecified regularization of the perturbed regularized kernel of the fermionic projector from Definition 4.1.1 will be a deformed version of the iε-regularization widely and almost exclusively used in the literature. While we have not imposed many restrictions on the choice of the regularized kernel of the fermionic projector except for its vector-scalar structure, we now make the following assumptions.

Assumption 5.1.1 (Anisotropic Perturbation of iε-Regularization)

Throughout this chapter, we consider perturbed regularized kernels of the fermionic projector having vector-scalar structure as in (4.1) with the vector and scalar components in momentum space given by

$$\widehat{v^\varepsilon_{\tau,i}}(p) = p_i \delta\big(\sigma(p)\big)\Theta(-p^0)\mathrm{e}^{\varepsilon p^0 f_\tau(p)} \tag{5.1a}$$

$$\widehat{s^\varepsilon_\tau}(p) = \mu \delta\big(\sigma(p)\big)\Theta(-p^0)\mathrm{e}^{\varepsilon p^0 f_\tau(p)} \tag{5.1b}$$

The real-valued function f_τ is assumed to be an L^2-function with respect to its spatial arguments and to have a perturbation expansion in the parameter τ which is given by

$$f_\tau(p) = 1 + \sum_{n=1}^{\infty} \frac{\tau^n}{n!} f^{(n)}_{lm}(p^0, |\vec{p}|) Y_{lm}(\theta_p, \varphi_p) \tag{5.1c}$$

where we have decomposed the functions $f^{(n)}(p)$ into a multipole series. Note that we have replaced the deformed regularized mass shell σ^ε_τ from (4.2) by its unperturbed, unregularized counterpart $\sigma(p) := \sigma^0_0(p) = p^2 - \mu^2$.[a] For vanishing perturbation ($\tau = 0$), the regularization goes over to the ordinary iε-regularization.[b]

[a] As a consequence of the replacement $\sigma^\varepsilon_\tau(p) \to p^2 - \mu^2$, also the regularization-dependence of the vectors $(\Delta^{(n)})^\varepsilon_{lm}$ of multipole moments of variations of the regularized kernel of the fermionic projector disappears.

[b] A review of the iε-regularized kernel of the fermionic projector along with an explicit computation of its vector and scalar components can be found in Subsection 2.3.2.

This perturbed regularized kernel of the fermionic projector describes an iε-regularization for which the regularization length $\varepsilon(\vec{p})$ does not only depend on p^0 (as would be the case for the ordinary iε-regularization), but which depends on the position on the mass shell. Thus, the decay behavior of $\widehat{\mathrm{P}^\varepsilon}$ as modelled by the exponential factor has the same *overall* tendency, namely a stronger decay for higher frequencies, but with varying behaviour in different spatial directions.

5.1.1 Variation of $\widehat{\mathrm{P}^\varepsilon}$ for Anisotropic iε-Regularization

Having specified the regularization, we can now tackle the question how deformations of the regularized kernel of the fermionic projector around the spherically-symmetric configuration translate into variations of the regularized causal action at different multipole orders. To answer this question, we start by deriving the multipole moments $\Delta^{(n)}_{lm}$ of the regularized kernel of the fermionic projector in momentum space.

Lemma 5.1.2 (Multipole Expansion of Variations of $\widehat{\mathrm{P}^\varepsilon}$ from Assumption 5.1.1)

The multipole moments of the variation of the regularized kernel of the fermionic projector as given in Assumption 5.1.1 read

$$\Delta_{lm}(p^0, |\vec{p}|) = (\varepsilon p^0) f^{(1)}_{lm}(p^0, |\vec{p}|)\mathrm{e}^{\varepsilon p^0} \begin{pmatrix} p^0 & |\vec{p}| & 0 & 0 & \mu \end{pmatrix}^{\mathrm{T}} \tag{5.2a}$$

$$(\Delta^2)_{lm}(p^0,|\vec{p}|) = \frac{1}{2}\Big[(\varepsilon p^0) f^{(2)}_{lm}(p^0,|\vec{p}|) + (\varepsilon p^0)^2 f^{(1,1)}_{lm}(p^0,|\vec{p}|)\Big] \mathrm{e}^{\varepsilon p^0} \begin{pmatrix} p^0 & |\vec{p}| & 0 & 0 & \mu \end{pmatrix}^{\mathrm{T}} \tag{5.2b}$$

where the functions $f^{(1,1)}_{lm}$ for $(l,m) \in \mathbb{N}_0 \times \mathbb{Z}$ with $-l \leq m \leq l$ are given in terms of Wigner's 3j-symbols by

$$f^{(1,1)}_{lm}(p^0,|\vec{p}|) = \sum_{l_1,m_1}\sum_{l_2,m_2} f^{(1)}_{l_1m_1}(p^0,|\vec{p}|) f^{(1)}_{l_2m_2}(p^0,|\vec{p}|) \sqrt{\frac{(2l+1)(2l_1+1)(2l_2+1)}{4\pi}} \times$$
$$\times (-1)^m \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & m \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \tag{5.2b,i}$$

Proof. By expanding the anisotropically iε-regularized kernel of the fermionic projector with respect to the perturbation parameter τ, we obtain

$$\widehat{\mathrm{P}^\varepsilon_\tau}(p) = \widehat{\mathrm{P}^\varepsilon_0}(p) + \tau\delta\widehat{\mathrm{P}^\varepsilon}(p) + \tau^2\delta^2\widehat{\mathrm{P}^\varepsilon}(p) + \mathcal{O}(\tau^3) \tag{5.3}$$

where the first-order variation is given by

$$\begin{aligned}
\delta\widehat{\mathrm{P}^\varepsilon}(p) &= \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}\tau}\Big[(p^0\gamma^0 - \vec{p}\vec{\gamma} + \mu\,\mathrm{id}_{\mathbb{C}^4})\mathrm{e}^{\varepsilon p^0 f_\tau(p)}\delta(p^2-\mu^2)\Theta(-p^0)\Big]\Big|_{\tau=0} \\
&= \sum_{l,m}(p^0\gamma^0 - \vec{p}\vec{\gamma} + \mu\,\mathrm{id}_{\mathbb{C}^4})\varepsilon p^0 f^{(1)}_{lm}(p^0,|\vec{p}|) Y_{lm} \mathrm{e}^{\varepsilon p^0}\delta(p^2-\mu^2)\Theta(-p^0) \\
&= \sum_{l,m}\varepsilon p^0 f^{(1)}_{lm}(p^0,|\vec{p}|) Y_{lm}\widehat{\mathrm{P}^\varepsilon_0}(p)
\end{aligned} \tag{5.4}$$

while the second-order variation reads

$$\begin{aligned}
\delta^2\widehat{\mathrm{P}^\varepsilon}(p) &= \frac{1}{2!}\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}\Big[(p^0\gamma^0 - \vec{p}\vec{\gamma} + \mu\,\mathrm{id}_{\mathbb{C}^4})\mathrm{e}^{\varepsilon p^0 f_\tau(p)}\delta(p^2-\mu^2)\Theta(-p^0)\Big]\Big|_{\tau=0} \\
&= \frac{(p^0\gamma^0 - \vec{p}\vec{\gamma} + \mu\,\mathrm{id}_{\mathbb{C}^4})}{2}\delta(p^2-\mu^2)\Theta(-p^0)\times \\
&\quad\times\Bigg[\sum_{l_1,m_1}\varepsilon p^0\Big(f^{(2)}_{l_1m_1}(p^0,|\vec{p}|)Y_{l_1m_1} + \mathcal{O}(\tau)\Big)\mathrm{e}^{\varepsilon p^0 f_\tau(p)} \\
&\qquad + \sum_{l_1,m_1}\sum_{l_2,m_2}(\varepsilon p^0)^2\Big(f^{(1)}_{l_1m_1}(p^0,|\vec{p}|)Y_{l_1m_1} + \tau f^{(2)}_{l_1m_1}(p^0,|\vec{p}|)Y_{l_1m_1} + \mathcal{O}(\tau^2)\Big)\times \\
&\qquad\qquad\times\Big(f^{(1)}_{l_2m_2}(p^0,|\vec{p}|)Y_{l_2m_2} + \tau f^{(2)}_{l_2m_2}(p^0,|\vec{p}|)Y_{l_2m_2} + \mathcal{O}(\tau^2)\Big)\mathrm{e}^{\varepsilon p^0 f_\tau(p)}\Bigg]\Bigg|_{\tau=0} \\
&= \frac{\varepsilon p^0}{2}\sum_{l_1,m_1}\Bigg[f^{(2)}_{l_1m_1}(p^0,|\vec{p}|)Y_{l_1m_1} \\
&\qquad + \sum_{l_2,m_2}(\varepsilon p^0) f^{(1)}_{l_1m_1}(p^0,|\vec{p}|) f^{(1)}_{l_2,m_2}(p^0,|\vec{p}|)Y_{l_1m_1}Y_{l_2m_2}\Bigg]\widehat{\mathrm{P}^\varepsilon_0}(p)
\end{aligned} \tag{5.5}$$

In order to obtain an expression which is proportional to only one spherical harmonic, we make use of the following identity for the product of two spherical harmonics[78, p. 146],[a]

$$\begin{aligned}
Y_{l_1m_1}(\theta,\varphi)Y_{l_2m_2}(\theta,\varphi) &= \sqrt{\frac{(1+2l_1)(1+2l_2)(1+2l)}{4\pi}}\times \\
&\quad\times\sum_{l,m}(-1)^m\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}\begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} Y_{lm}(\theta,\varphi)
\end{aligned} \tag{5.6}$$

where the admissible values for l, m are determined by the selection rules of Wigner's $3j$-symbols which read

$$-l_i \leq m_i \leq l_i, \qquad -l \leq m \leq l, \qquad m = -(m_1 + m_2), \qquad |l_1 - l_2| \leq l \leq l_1 + l_2 \tag{5.7}$$

By defining

$$f^{(1,1)}_{lm}(p^0, |\vec{p}|) := \sum_{l_1, m_1} \sum_{l_2, m_2} f^{(1)}_{l_1 m_1}(p^0, |\vec{p}|) f^{(1)}_{l_2 m_2}(p^0, |\vec{p}|) \sqrt{\frac{(1+2l_1)(1+2l_2)(1+2l)}{4\pi}} \times \\ \times (-1)^m \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \tag{5.8}$$

the second variation thus takes the form

$$\delta^2 \widehat{\mathrm{P}^\varepsilon}(p) = \frac{1}{2} \sum_{l,m} \Big[(\varepsilon p^0) f^{(2)}_{lm}(p^0, |\vec{p}|) + (\varepsilon p^0)^2 f^{(1,1)}_{lm}(p^0, |\vec{p}|) \Big] Y_{lm}(\theta_p, \varphi_p) \widehat{\mathrm{P}^\varepsilon_0}(p) \tag{5.9}$$

Decomposing (5.4) and (5.9) into vector spherical harmonics in the same way as in the paragraph following Definition 4.1.3, we immediately recognize that due to the choice $\widehat{v^\varepsilon_{\tau,i}}(p) \propto p_i$ in (5.1a), terms proportional to $\vec{\Psi}_{lm}$ and $\vec{\Phi}_{lm}$ are absent. As a consequence we end up with

$$\Delta_{lm}(p^0, |\vec{p}|) = (\varepsilon p^0) f^{(1)}_{lm}(p^0, |\vec{p}|) \mathrm{e}^{\varepsilon p^0} \begin{pmatrix} p^0 & |\vec{p}| & 0 & 0 & \mu \end{pmatrix}^{\mathrm{T}} \tag{5.10a}$$

$$(\Delta^2)_{lm}(p^0, |\vec{p}|) = \frac{1}{2} \Big[(\varepsilon p^0) f^{(2)}_{lm}(p^0, |\vec{p}|) + (\varepsilon p^0)^2 f^{(1,1)}_{lm}(p^0, |\vec{p}|) \Big] \mathrm{e}^{\varepsilon p^0} \begin{pmatrix} p^0 & |\vec{p}| & 0 & 0 & \mu \end{pmatrix}^{\mathrm{T}} \tag{5.10b}$$

which concludes the proof. □

[a] We remark that the convention for the spherical harmonics as used by Brink and Satchler[78, p. 145] is compatible with Definition 4.1.3.

5.1.2 Variation of $\mathcal{S}^\varepsilon$ for Anisotropic iε-Regularization

Having derived the five-component vector of multipole moments of variations of an anisotropically iε-regularized kernel of the fermionic projector, we can now customize the expression for the multipole moments of the variation of the regularized causal action as derived in Theorem 4.3.1 to this special setting. Before, however, we exploit the fact that the multipole moments Δ_{lm} and $(\Delta^2)_{lm}$ in (5.2a) and (5.2b) are all proportional to the same vector by introducing so-called *condensed incomplete Fourier transforms* which turn the matrix-valued incomplete Fourier transforms into scalar-valued functions.

Definition 5.1.3 (Condensed Incomplete Fourier Transforms)

For $(\,\bullet\,) \in \{\mathcal{M}^\varepsilon, \mathcal{N}^\varepsilon, \mathcal{V}^\varepsilon, \mathcal{W}^\varepsilon\}$ the *condensed incomplete Fourier transforms* $\{\mathcal{F}\big[(\,\bullet\,)^\varepsilon_{lm|l'm'}\big]\}$ are defined as

$$\Big\{ \mathcal{F}\big[(\,\bullet\,)^\varepsilon_{lm|l'm'}\big] \Big\} := \begin{pmatrix} p^0 & |\vec{p}| & 0 & 0 & \mu \end{pmatrix} \mathcal{F}\big[(\,\bullet\,)^\varepsilon_{lm|l'm'}\big] \begin{pmatrix} q^0 & |\vec{q}| & 0 & 0 & \mu \end{pmatrix}^{\mathrm{T}} \tag{5.11}$$

where $\mathcal{M}^\varepsilon, \mathcal{N}^\varepsilon, \mathcal{V}^\varepsilon, \mathcal{W}^\varepsilon$ are the incomplete Fourier transforms defined in Definition 4.2.1. Analogously, we define for the incomplete Fourier transform $\mathcal{K}^\varepsilon_{lm}$

$$\Big\{ \mathcal{F}\big[\mathcal{K}^\varepsilon_{lm}\big] \Big\} := \mathbb{1}_{1\times 5}\, \mathcal{F}\big[\mathcal{K}^\varepsilon_{lm}\big] \begin{pmatrix} p^0 & |\vec{p}| & 0 & 0 & \mu \end{pmatrix}^{\mathrm{T}} \tag{5.12}$$

Using this definition and the explicit form of the multipole moments Δ_{lm} and $(\Delta^2)_{lm}$ from Lemma 5.1.2 it is now possible, starting from Theorem 4.3.1, to derive expressions for the multipole moments of the variation of the regularized causal action in which the occurring integral operators no longer have matrix-valued, but only scalar-valued integral kernels.

Theorem 5.1.4 (Variation of the Regularized Causal Action for Lemma 5.1.2)

The variation of the regularized causal action corresponding to an anisotropically iε-regularized kernel of the fermionic projector as given in Assumption 5.1.1 takes the form

$$\delta\mathcal{S}^\varepsilon = \mathrm{Re}\left[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\; Q_0(|\vec{p}|) f_{00}^{(1)}(|\vec{p}|)\right] \tag{5.13a}$$

$$\delta^2\mathcal{S}^\varepsilon = \mathrm{Re}\left[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\;\frac{Q_0^\varepsilon(|\vec{p}|)}{2} f_{00}^{(2)}(|\vec{p}|) + \frac{1}{2}\sum_{l,m}\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\; f_{lm}^{(1)}(|\vec{p}|) Q_{lm}^\varepsilon(|\vec{p}|,|\vec{q}|)\overline{f_{lm}^{(1)}(|\vec{q}|)}\right] \tag{5.13b}$$

where the scalar-valued integral kernels are given by

$$Q_0^\varepsilon(|\vec{p}|) = -\varepsilon\omega_p \mathrm{e}^{-\varepsilon\omega_p}\;\Big\{\mathcal{F}\big[\mathcal{K}_{00}^\varepsilon\big](|\vec{p}|)\Big\} \tag{5.13a,i}$$

$$\begin{aligned} Q_{lm}^\varepsilon(|\vec{p}|,|\vec{q}|) = &-\frac{\varepsilon\omega_p Q_0^\varepsilon(|\vec{p}|)}{\sqrt{4\pi}}\frac{(2\pi)^4}{|\vec{q}|^2}\delta(|\vec{p}|-|\vec{q}|) + \varepsilon^2\omega_p\omega_q \mathrm{e}^{-\varepsilon(\omega_p+\omega_q)}\times \\ &\times\Big(\Big\{\mathcal{F}\big[\mathcal{M}_{l0|l0}^\varepsilon\big](|\vec{p}|,|\vec{q}|)\Big\} + \Big\{\mathcal{F}\big[\mathcal{N}_{l0|l0}^\varepsilon\big](|\vec{p}|,|\vec{q}|)\Big\} \\ &-\Big\{\mathcal{F}\big[\mathcal{V}_{l0|l0}^\varepsilon\big](|\vec{p}|,|\vec{q}|)\Big\} - \Big\{\mathcal{F}\big[\mathcal{W}_{l0|l0}^\varepsilon\big](|\vec{p}|,|\vec{q}|)\Big\}\Big) \end{aligned} \tag{5.13b,i}$$

Proof. In order to derive the claimed expressions for the variation of the regularized causal action, we basically have to insert (5.2a) and (5.2b) into (4.51a) and (4.51b), respectively, and make use of Definition 5.1.3.

(1) Multipole Moments of $\delta\mathcal{S}^\varepsilon$

According to Theorem 4.3.1, the only non-vanishing multipole moment of $\delta\mathcal{S}^\varepsilon$ is the one for $l=0$. Inserting (5.2a) into (4.51a) thus yields

$$\begin{aligned} \delta\mathcal{S}_0^\varepsilon &\overset{(4.51a)}{=} \mathrm{Re}\left[\left\langle\!\!\left\langle \mathbb{1}_{5\times 1}, \mathrm{R}_{00}^\varepsilon\Delta_{00}\right\rangle\!\!\right\rangle\right] \\ &\overset{(5.2a)}{\underset{(5.11)}{=}} \mathrm{Re}\left[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\;\Big\{\mathcal{F}\big[\mathcal{K}_{00}^\varepsilon\big](|\vec{p}|)\Big\}\big(-\varepsilon\omega_p\big)\overline{f_{00}^{(1)}\big(-\omega_p,|\vec{p}|\big)}\mathrm{e}^{-\varepsilon\omega_p}\right] \\ &= \mathrm{Re}\left[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\; Q_0^\varepsilon(|\vec{p}|) f_{00}^{(1)}\big(-\omega_p,|\vec{p}|\big)\right] \end{aligned}$$

where we used the relation $\overline{f_{00}^{(1)}} = f_{00}^{(1)}$ and where the scalar-valued integral kernel Q_0^ε is defined as

$$Q_0^\varepsilon(|\vec{p}|) := -\varepsilon\omega_p \mathrm{e}^{-\varepsilon\omega_p}\Big\{\mathcal{F}\big[\mathcal{K}_{00}^\varepsilon\big](|\vec{p}|)\Big\}$$

with $\{\mathcal{F}[\mathcal{K}^{\varepsilon}_{00}]\}$ denoting the condensed incomplete Fourier transform of $\mathcal{F}[\mathcal{K}^{\varepsilon}_{00}]$ as given in (4.44a). To simplify notation, we replace $f^{(n)}_{lm}(-\omega_p, |\vec{p}|)$ by $f^{(n)}_{lm}(|\vec{p}|)$ from now on whenever there is no risk of confusion.

(2) Multipole Moments of $\delta^2\mathcal{S}^{\varepsilon}$

For the second variation the procedure is basically the same, though slightly more involved due to the fact that there are two terms in (4.51b): On the one hand there is the term depending linearly on the second variation Δ^2 while on the other hand there is the sesquilinear term which involves the first variation Δ twice.

(a) Linear Term (only present for $l = 0$)

We start by considering the former contribution, namely the one which involves the second-order variation of the regularized kernel of the fermionic projector. Inserting (5.2b) into the first term in (4.51b) yields

$$\delta^2\mathcal{S}^{\varepsilon}_{\text{lin}} \overset{(4.51b)}{=} \mathrm{Re}\left[\left\langle\!\!\left\langle \mathbb{1}_{5\times 1}, \mathrm{R}^{\varepsilon}_{00}(\Delta^2)_{00}\right\rangle\!\!\right\rangle\right]$$
$$\underset{(5.11)}{\overset{(5.2b)}{=}} \mathrm{Re}\left[\int_0^{\infty} \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4} \left\{\mathcal{F}[\mathcal{K}^{\varepsilon}_{00}](|\vec{p}|)\right\}\frac{1}{2}\left[\big(-\varepsilon\omega_p\big)\overline{f^{(2)}_{00}(|\vec{p}|)} + \big(\varepsilon\omega_p\big)^2\overline{f^{(1,1)}_{00}(|\vec{p}|)}\right]\mathrm{e}^{-\varepsilon\omega_p}\right]$$

Recalling the definition of the functions $f^{(1,1)}_{lm}$ from (5.2b,i), choosing $l = m = 0$ and employing the simplified notation where $f^{(n)}_{lm}(-\omega_p, |\vec{p}|)$ is abbreviated by $f^{(n)}_{lm}(|\vec{p}|)$, we find

$$\begin{aligned} f^{(1,1)}_{00}(|\vec{p}|) &\overset{(5.2b,i)}{=} \sum_{l_1,m_1}\sum_{l_2,m_2} f^{(1)}_{l_1m_1}(|\vec{p}|)f^{(1)}_{l_2m_2}(|\vec{p}|)\sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi}}\times \\ &\qquad\times\begin{pmatrix} l_1 & l_2 & 0 \\ m_1 & m_2 & 0\end{pmatrix}\begin{pmatrix} l_1 & l_2 & 0 \\ 0 & 0 & 0\end{pmatrix} \\ &= \sum_{l_1,m_1}\sum_{l_2,m_2} f^{(1)}_{l_1m_1}(|\vec{p}|)f^{(1)}_{l_2m_2}(|\vec{p}|)\sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi}}\times \\ &\qquad\times\left(\frac{(-1)^{l_1-m_1}}{\sqrt{1+2l_1}}\right)\left(\frac{(-1)^{l_1}}{\sqrt{1+2l_1}}\right)\delta_{l_1l_2}\delta_{m_1(-m_2)} \\ &= \frac{1}{\sqrt{4\pi}}\sum_{l_1,m_1}(-1)^{-m_1}f^{(1)}_{l_1m_1}(|\vec{p}|)f^{(1)}_{l_1(-m_1)}(|\vec{p}|) \\ &= \frac{1}{\sqrt{4\pi}}\sum_{l_1,m_1} f^{(1)}_{l_1m_1}(|\vec{p}|)\overline{f^{(1)}_{l_1m_1}(|\vec{p}|)} \end{aligned}$$

Here we used the relation $\overline{f^{(n)}_{lm}(|\vec{q}|)} = (-1)^m f^{(n)}_{l(-m)}(|\vec{q}|)$ for the coefficient functions in the multipole expansion of a real-valued function in the last step. For the second equality we evaluated Wigner's 3j-symbols using formulas provided by Brink and Satchler[78, p. 138]. In this way we find that $\delta^2\mathcal{S}^{\varepsilon}_{\text{lin}}$ actually contains functions $f^{(1)}_{\tilde{l}\tilde{m}}$ of arbitrary high multipole orders $\tilde{l} \in \mathbb{N}_0$ and takes the form

$$\delta^2\mathcal{S}^{\varepsilon}_{\text{lin}} = \delta^2\mathcal{S}^{\varepsilon}_{\text{lin},0}\left[f^{(2)}_{00}, f^{(1)}_{00}\right] + \sum_{\tilde{l}=1}^{\infty}\delta^2\mathcal{S}^{\varepsilon}_{\text{lin},\tilde{l}}\left[f^{(1)}_{\tilde{l}\tilde{m}}\right] \tag{5.14}$$

where the terms at lowest ($\tilde{l} = 0$) and higher ($\tilde{l} \geq 1$) multipole orders are given by

$$\delta^2 \mathcal{S}^{\varepsilon}_{\text{lin}}\left[f^{(2)}_{00}, f^{(1)}_{00}\right] = \text{Re}\left[\int_0^\infty \frac{\text{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\left(\frac{Q^{\varepsilon}_0(|\vec{p}|)}{2} f^{(2)}_{00}(|\vec{p}|) + f^{(1)}_{00}(|\vec{p}|)\left(-\varepsilon\frac{\omega_p Q^{\varepsilon}_0(|\vec{p}|)}{\sqrt{16\pi}}\right)\overline{f^{(1)}_{00}(|\vec{p}|)}\right)\right]$$

$$\delta^2 \mathcal{S}^{\varepsilon}_{\text{lin},\tilde{l}}\left[f^{(1)}_{\tilde{l}\tilde{m}}\right] = \text{Re}\left[\sum_{\tilde{m}=-\tilde{l}}^{\tilde{l}} \int_0^\infty \frac{\text{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\; f^{(1)}_{\tilde{l}\tilde{m}}(|\vec{p}|)\left(-\varepsilon\frac{\omega_p Q^{\varepsilon}_0(|\vec{p}|)}{\sqrt{16\pi}}\right)\overline{f^{(1)}_{\tilde{l}\tilde{m}}(|\vec{p}|)}\right]$$

respectively. We remark that the tildes are added in order to clarify that, although the linear term is present only for $l = 0$, we nevertheless obtain higher-order multipole contributions which are "hidden" inside $f^{(1,1)}_{00}$.

(b) Sesquilinear Term

In contrast with the linear term, the sesquilinear term is not only present at multipole order $l = 0$, but for arbitrary $l \in \mathbb{N}_0$. Proceeding in exactly the same way as before by inserting (5.2a) into the second term in (4.51b) we thus obtain

$$\begin{aligned}
\delta^2 \mathcal{S}^{\varepsilon}_{\text{sql},l} &\overset{(4.51b)}{=} \text{Re}\left[\frac{1}{2}\sum_{m=-l}^{l}\left\langle\!\!\left\langle \Delta_{lm}, \text{S}^{\varepsilon}_{lm}\Delta_{lm}\right\rangle\!\!\right\rangle\right] \\
&\overset{(5.2a)}{\underset{(5.11)}{=}} \sum_{m=-l}^{l}\text{Re}\left[\frac{1}{2}\int_0^\infty \frac{\text{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\int_0^\infty \frac{\text{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\;\varepsilon^2\omega_p\omega_q \text{e}^{-\varepsilon\omega_p}\text{e}^{-\varepsilon\omega_q} f^{(1)}_{lm}(|\vec{p}|)\overline{f^{(1)}_{lm}(|\vec{q}|)}\times\right. \\
&\quad\times\left((-1)^{-m}\left\{\mathcal{F}\left[\mathcal{M}^{\varepsilon}_{lm|l(-m)}\right](|\vec{p}|,|\vec{q}|)\right\} - (-1)^{-m}\left\{\mathcal{F}\left[\mathcal{V}^{\varepsilon}_{lm|l(-m)}\right](|\vec{p}|,|\vec{q}|)\right\}\right. \\
&\quad\left.\left. +\left\{\mathcal{F}\left[\mathcal{N}^{\varepsilon}_{lm|l(-m)}\right](|\vec{p}|,|\vec{q}|)\right\} - \left\{\mathcal{F}\left[\mathcal{W}^{\varepsilon}_{lm|l(-m)}\right](|\vec{p}|,|\vec{q}|)\right\}\right)\right]
\end{aligned}$$

To simplify this expression we recall that according to Lemma 4.2.12 we have

$$\mathcal{F}\left[\mathcal{M}^{\varepsilon}_{lm|l(-m)}\right] = (-1)^m\mathcal{F}\left[\mathcal{M}^{\varepsilon}_{l0|l0}\right] \qquad \mathcal{F}\left[\mathcal{N}^{\varepsilon}_{lm|l(-m)}\right] = \mathcal{F}\left[\mathcal{N}^{\varepsilon}_{l0|l0}\right]$$
$$\mathcal{F}\left[\mathcal{V}^{\varepsilon}_{lm|l(-m)}\right] = (-1)^m\mathcal{F}\left[\mathcal{V}^{\varepsilon}_{l0|l0}\right] \qquad \mathcal{F}\left[\mathcal{W}^{\varepsilon}_{lm|l(-m)}\right] = \mathcal{F}\left[\mathcal{W}^{\varepsilon}_{l0|l0}\right]$$

Using the relation $\overline{f^{(n)}_{lm}(|\vec{q}|)} = (-1)^m f^{(n)}_{l(-m)}(|\vec{q}|)$ once more allows to combine terms such that we arrive at

$$\begin{aligned}
\delta^2 \mathcal{S}^{\varepsilon}_{\text{sql},l} = \sum_{m=-l}^{l}\text{Re}&\left[\frac{1}{2}\int_0^\infty \frac{\text{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\int_0^\infty \frac{\text{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\;\varepsilon^2\omega_p\omega_q \text{e}^{-\varepsilon\omega_p}\text{e}^{-\varepsilon\omega_q}\times\right. \\
&\times f^{(1)}_{lm}(|\vec{p}|)\left(\left\{\mathcal{F}\left[\mathcal{M}^{\varepsilon}_{l0|l0}\right](|\vec{p}|,|\vec{q}|)\right\} + \left\{\mathcal{F}\left[\mathcal{N}^{\varepsilon}_{l0|l0}\right](|\vec{p}|,|\vec{q}|)\right\}\right. \\
&\left.\left. - \left\{\mathcal{F}\left[\mathcal{V}^{\varepsilon}_{l0|l0}\right](|\vec{p}|,|\vec{q}|)\right\} - \left\{\mathcal{F}\left[\mathcal{W}^{\varepsilon}_{l0|l0}\right](|\vec{p}|,|\vec{q}|)\right\}\right)\overline{f^{(1)}_{lm}(|\vec{q}|)}\right]
\end{aligned}$$

(3) Conclusion
Adding up the linear and sesquilinear contributions of the second variation of the regularized causal action, we arrive at the following expression

$$\delta^2\mathcal{S}^\varepsilon = \mathrm{Re}\Bigg[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\,\frac{Q_0^\varepsilon(|\vec{p}|)}{2}\,f_{00}^{(2)}(|\vec{p}|) + \frac{1}{2}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\; f_{lm}^{(1)}(|\vec{p}|)Q_{lm}^\varepsilon(|\vec{p}|,|\vec{q}|)\overline{f_{lm}^{(1)}(|\vec{q}|)}\Bigg]$$

where for all $(l,m)\in\mathbb{N}_0\times\mathbb{Z}$ with $-l\le m\le l$ the scalar-valued integral kernels $Q_{lm}^\varepsilon(|\vec{p}|,|\vec{q}|)$ are given by

$$\begin{aligned}Q_{lm}^\varepsilon(|\vec{p}|,|\vec{q}|) = &-\frac{\varepsilon\omega_p Q_0^\varepsilon(|\vec{p}|)}{\sqrt{4\pi}}\,\frac{(2\pi)^4}{|\vec{q}|^2}\,\delta(|\vec{p}|-|\vec{q}|)\\ &+\varepsilon^2\omega_p\omega_q e^{-\varepsilon(\omega_p+\omega_q)}\Big(\Big\{\mathcal{F}\big[\mathcal{M}_{l0|l0}^\varepsilon\big](|\vec{p}|,|\vec{q}|)\Big\}+\Big\{\mathcal{F}\big[\mathcal{N}_{l0|l0}^\varepsilon\big](|\vec{p}|,|\vec{q}|)\Big\}\\ &\qquad-\Big\{\mathcal{F}\big[\mathcal{V}_{l0|l0}^\varepsilon\big](|\vec{p}|,|\vec{q}|)\Big\}-\Big\{\mathcal{F}\big[\mathcal{W}_{l0|l0}^\varepsilon\big](|\vec{p}|,|\vec{q}|)\Big\}\Big)\end{aligned}$$

This concludes the proof. □

Starting from this expression, we demonstrate in the next section the invariance of the regularized causal action under Lorentz boosts of the velocity vector of the iε-regularization. Afterwards we study so-called *compensations*, which counterbalance initial perturbations and thus leave the regularized causal action unchanged. Also for the next chapter, in which we study the invertibility of the second variation of the regularized causal action, Theorem 5.1.4 will be the starting point.

5.2 Invariance of $\mathcal{S}^\varepsilon$ under Lorentz Boosts

In this section, we study the effect of Lorentz boosts on the regularized causal action with iε-regularization and demonstrate, by using the above Theorem 5.1.4, that it is invariant.

5.2.1 Derivation of the Variation of $\widehat{\mathrm{P}^\varepsilon}$ for Lorentz Boosts

To prove invariance of the iε-regularized causal action under Lorentz boosts of the velocity vector of the regularization, we first derive the multipole expansion of the corresponding variation of the regularized kernel of the fermionic projector and subsequently show that the variation of the regularized causal action as derived in Theorem 5.1.4 vanishes for these variations.

Lemma 5.2.1 (Multipole Expansion of the Variation of $\widehat{\mathrm{P}^\varepsilon}$ for Lorentz Boosts)

Let $\widehat{\mathrm{P}_0^\varepsilon}(p)$ be an unperturbed regularized kernel of the fermionic projector as given in Assumption 5.1.1 (for $\tau=0$) with the vector and scalar components taking the form

$$\widehat{v_0^\varepsilon}(p) = p^0\delta\big(\sigma(p)\big)\Theta(-p^0)e^{\varepsilon pu} \tag{5.16a}$$
$$\widehat{v_\alpha^\varepsilon}(p) = -p^\alpha\delta\big(\sigma(p)\big)\Theta(-p^0)e^{\varepsilon pu} \tag{5.16b}$$
$$\widehat{s^\varepsilon}(p) = \mu\delta\big(\sigma(p)\big)\Theta(-p^0)e^{\varepsilon pu} \tag{5.16c}$$

where $u=(1,0,0,0)$ denotes the four-velocity of the regularization. Under a Lorentz boost of this four-velocity in direction $\vec{n}$, the non-vanishing multipole moments of the first and second variation of $\widehat{\mathrm{P}^\varepsilon}(p)$ are given by

$$\Delta_{1m}(p^0,|\vec{p}|) = \varepsilon|\vec{p}|\mathrm{e}^{\varepsilon p^0}\sqrt{\frac{4\pi}{3}}\begin{pmatrix} p^0 \\ |\vec{p}| \\ 0 \\ 0 \\ \mu \end{pmatrix} \times \begin{cases} n^3 & \text{for } m = 0 \\ \mp\frac{n^1\mp in^2}{\sqrt{2}} & \text{for } m = \pm 1 \end{cases} \tag{5.17a}$$

$$(\Delta^2)_{00}(p^0,|\vec{p}|) = \sqrt{\pi}\left[\varepsilon p^0 + \frac{1}{3}\varepsilon^2|\vec{p}|^2\right]\mathrm{e}^{\varepsilon p^0}\begin{pmatrix} p^0 \\ |\vec{p}| \\ 0 \\ 0 \\ \mu \end{pmatrix} \tag{5.17b}$$

$$(\Delta^2)_{2m}(p^0,|\vec{p}|) = \sqrt{\frac{\pi}{30}}\varepsilon^2|\vec{p}|^2\mathrm{e}^{\varepsilon p^0}\begin{pmatrix} p^0 \\ |\vec{p}| \\ 0 \\ 0 \\ \mu \end{pmatrix} \times \begin{cases} \sqrt{\frac{2}{3}}\left[3(n^3)^2 - 1\right] & \text{for } m = 0 \\ \pm 2(n^1 \pm \mathrm{i}n^2)n^3 & \text{for } m = \pm 1 \\ (n^1 \pm \mathrm{i}n^2)^2 & \text{for } m = \pm 2 \end{cases} \tag{5.17c}$$

Proof. Acting with a Lorentz boost in direction $\vec{n} \in \mathbb{R}^3$ which is explicitly given by

$$u \mapsto B_\zeta(u) := \begin{pmatrix} u^0\cosh(\zeta) - \sinh(\zeta)\vec{n}\cdot\vec{u} \\ \vec{u} - (\vec{n}\cdot\vec{u})\vec{n} + \left[\cosh(\zeta)(\vec{n}\cdot\vec{u}) - \sinh(\zeta)u^0\right]\vec{n} \end{pmatrix} \tag{5.18}$$

on the velocity vector of the regularized kernel of the fermionic projector as given in Assumption 5.1.1 and expanding the result with respect to the boost parameter ζ, we obtain

$$\widehat{\mathrm{P}^\varepsilon_\zeta}(p) = \widehat{\mathrm{P}^\varepsilon_0}(p) + \zeta\delta\widehat{\mathrm{P}^\varepsilon}(p) + \zeta^2\delta^2\widehat{\mathrm{P}^\varepsilon}(p) + \mathcal{O}(\zeta^3) \tag{5.19}$$

where the variations at first and second order are given by

$$\begin{aligned}
\delta\widehat{\mathrm{P}^\varepsilon}(p) &= \frac{1}{1!}\frac{\mathrm{d}}{\mathrm{d}\zeta}\left[\left(p^0\gamma^0 - \vec{p}\vec{\gamma} + \mu\,\mathrm{id}_{\mathbb{C}^4}\right)\mathrm{e}^{\varepsilon pB_\zeta(u)}\delta\big(\sigma(p)\big)\Theta(-p^0)\right]\Bigg|_{\zeta=0} \\
&= \left[\left(p^0\gamma^0 - \vec{p}\vec{\gamma} + \mu\,\mathrm{id}_{\mathbb{C}^4}\right)\left(\varepsilon p^0\sinh(\zeta) + \varepsilon\vec{p}\cdot\vec{n}\cosh(\zeta)\right)\mathrm{e}^{\varepsilon pB_\zeta(u)}\delta\big(\sigma(p)\big)\Theta(-p^0)\right]\Bigg|_{\zeta=0} \\
&= \left(p^0\gamma^0 - \vec{p}\vec{\gamma} + \mu\,\mathrm{id}_{\mathbb{C}^4}\right)\varepsilon(\vec{p}\cdot\vec{n})\mathrm{e}^{\varepsilon p^0}\delta\big(\sigma(p)\big)\Theta(-p^0) \\
&= \varepsilon(\vec{p}\cdot\vec{n})\widehat{\mathrm{P}^\varepsilon}(p)
\end{aligned} \tag{5.20}$$

and

$$\begin{aligned}
\delta^2\widehat{\mathrm{P}^\varepsilon}(p) &= \frac{1}{2!}\frac{\mathrm{d}^2}{\mathrm{d}\zeta^2}\left[\left(p^0\gamma^0 - \vec{p}\vec{\gamma} + \mu\,\mathrm{id}_{\mathbb{C}^4}\right)\mathrm{e}^{\varepsilon pB_\zeta(u)}\delta\big(\sigma(p)\big)\Theta(-p^0)\right]\Bigg|_{\zeta=0} \\
&= \frac{1}{2}\Big[\left(p^0\gamma^0 - \vec{p}\vec{\gamma} + \mu\,\mathrm{id}_{\mathbb{C}^4}\right)\left(\varepsilon p^0\cosh(\zeta) + \varepsilon\vec{p}\cdot\vec{n}\sinh(\zeta)\right)\mathrm{e}^{\varepsilon pB_\zeta(u)}\delta\big(\sigma(p)\big)\Theta(-p^0) \\
&\qquad + \left(p^0\gamma^0 - \vec{p}\vec{\gamma} + \mu\,\mathrm{id}_{\mathbb{C}^4}\right)\left(\varepsilon p^0\sinh(\zeta) + \varepsilon\vec{p}\cdot\vec{n}\cosh(\zeta)\right)^2\mathrm{e}^{\varepsilon pB_\zeta(u)}\delta\big(\sigma(p)\big)\Theta(-p^0)\Big]\Bigg|_{\zeta=0} \\
&= \frac{1}{2}\left(\varepsilon p^0 + \varepsilon^2(\vec{p}\cdot\vec{n})^2\right)\widehat{\mathrm{P}^\varepsilon}(p)
\end{aligned} \tag{5.21}$$

respectively. In order to find the multipole expansions of $\delta\widehat{\mathrm{P}^\varepsilon}(p)$ and $\delta^2\widehat{\mathrm{P}^\varepsilon}(p)$, we have to expand the scalar product $\vec{p}\cdot\vec{n}$ in spherical harmonics. To this end, we make use of the relation

$$\vec{p}\cdot\vec{n} = n^1|\vec{p}|\sin(\theta_p)\cos(\varphi_p) + n^2|\vec{p}|\sin(\theta_p)\sin(\varphi_p) + n^3|\vec{p}|\cos(\theta_p)$$

as well as

$$\sin(\theta_p)\begin{Bmatrix}\cos(\varphi_p)\\ \sin(\varphi_p)\end{Bmatrix} = \sqrt{\frac{2\pi}{3}}\begin{Bmatrix}-Y_{11}(\theta_p,\varphi_p)+Y_{1(-1)}(\theta_p,\varphi_p)\\ \mathrm{i}\big(Y_{11}(\theta_p,\varphi_p)+Y_{1(-1)}(\theta_p,\varphi_p)\big)\end{Bmatrix}$$

$$\cos(\theta_p) = \sqrt{\frac{4\pi}{3}}Y_{10}(\theta_p,\varphi_p)$$

for spherical harmonics at multipole order $l = 1$ and

$$\sin^2(\theta_p)\begin{Bmatrix}\cos^2(\varphi_p)\\ \sin^2(\varphi_p)\end{Bmatrix} = \frac{\sqrt{4\pi}}{3}\left(Y_{00}-\sqrt{\frac{1}{5}}Y_{20}\right)\pm\sqrt{\frac{2\pi}{15}}\big(Y_{22}+Y_{2(-2)}\big)$$

$$\sin^2(\theta_p)\sin(\varphi_p)\cos(\varphi_p) = -\mathrm{i}\sqrt{\frac{2\pi}{15}}\big(Y_{22}-Y_{2(-2)}\big)$$

$$\cos^2(\theta_p) = \frac{\sqrt{4\pi}}{3}\left(Y_{00}+\sqrt{\frac{4}{5}}Y_{20}\right)$$

$$\sin(\theta_p)\cos(\theta_p)\begin{Bmatrix}\cos(\varphi_p)\\ \sin(\varphi_p)\end{Bmatrix} = \sqrt{\frac{2\pi}{15}}\begin{Bmatrix}-Y_{21}+Y_{2(-1)}\\ \mathrm{i}\big(Y_{21}+Y_{2(-1)}\big)\end{Bmatrix}$$

for spherical harmonics at multipole order $l = 2$.

(1) Spherical Harmonic Expansion of $\delta\widehat{\mathrm{P}^\varepsilon}(p)$

For the first-order variation we obtain by using the above relations and sorting terms according to the different spherical harmonics

$$\begin{aligned}\delta\widehat{\mathrm{P}^\varepsilon}(p) &= \left(n^1\sqrt{\frac{2\pi}{3}}\big(-Y_{11}+Y_{1(-1)}\big)+\mathrm{i}n^2\sqrt{\frac{2\pi}{3}}\big(Y_{11}+Y_{1(-1)}\big)+n^3\sqrt{\frac{4\pi}{3}}Y_{10}\right)\varepsilon|\vec{p}|\widehat{\mathrm{P}^\varepsilon}(p)\\ &= \sqrt{\frac{4\pi}{3}}\left(-\frac{n^1-\mathrm{i}n^2}{\sqrt{2}}Y_{11}+\frac{n^1+\mathrm{i}n^2}{\sqrt{2}}Y_{1(-1)}+n^3Y_{10}\right)\varepsilon|\vec{p}|\widehat{\mathrm{P}^\varepsilon}(p)\end{aligned}$$

Inserting the vector-scalar form of the unperturbed regularized kernel of the fermionic projector, we obtain for the multipole moments $\Delta_{lm}(p^0,|\vec{p}|)$ at first order in perturbation theory

$$\Delta_{1m}(p^0,|\vec{p}|) = \varepsilon|\vec{p}|\mathrm{e}^{\varepsilon p^0}\sqrt{\frac{4\pi}{3}}\begin{pmatrix}p^0\\|\vec{p}|\\0\\0\\\mu\end{pmatrix}\times\begin{cases} n^3 & \text{for } m=0\\ \mp\frac{n^1\mp\mathrm{i}n^2}{\sqrt{2}} & \text{for } m=\pm1\end{cases} \tag{5.22}$$

while all other multipole moments for $l \neq 1$ vanish identically at first order.[a]

(2) Spherical Harmonic Expansion of $\delta^2\widehat{\mathrm{P}^\varepsilon}(p)$

For the variation at second order in perturbation theory, things are slightly more complicated due to the presence of the term $(\vec{p}\cdot\vec{n})^2$. Expanding the product $\vec{p}\cdot\vec{n}$ in the same way as before, taking the square and making use of linear combinations of spherical harmonics at $l = 2$ as derived above, we obtain

$$\begin{aligned}(\vec{p}\cdot\vec{n})^2 = |\vec{p}|^2\Big[&(n^1)^2\sin^2(\theta_p)\cos^2(\varphi_p)+(n^2)^2\sin^2(\theta_p)\sin^2(\varphi_p)+(n^3)^2\cos^2(\theta_p)\\ &+2n^1n^2\sin^2(\theta_p)\cos(\varphi_p)\sin(\varphi_p)+2n^1n^3\cos(\theta_p)\sin(\theta_p)\cos(\varphi_p)\\ &+2n^2n^3\cos(\theta_p)\sin(\theta_p)\sin(\varphi_p)\Big]\\ = |\vec{p}|^2\Bigg[&(n^1)^2\left[\frac{\sqrt{4\pi}}{3}\left(Y_{00}-\sqrt{\frac{1}{5}}Y_{20}\right)+\sqrt{\frac{2\pi}{15}}\big(Y_{22}+Y_{2(-2)}\big)\right]\end{aligned}$$

$$+ (n^2)^2\left[\frac{\sqrt{4\pi}}{3}\left(Y_{00} - \sqrt{\frac{1}{5}}Y_{20}\right) - \sqrt{\frac{2\pi}{15}}\big(Y_{22} + Y_{2(-2)}\big)\right]$$
$$+ (n^3)^2\left[\frac{\sqrt{4\pi}}{3}\left(Y_{00} + \sqrt{\frac{4}{5}}Y_{20}\right)\right] + 2n^1n^2\left[-\mathrm{i}\sqrt{\frac{2\pi}{15}}\big(Y_{22} - Y_{2(-2)}\big)\right]$$
$$+ 2n^1n^3\left[\sqrt{\frac{2\pi}{15}}\big(-Y_{21} + Y_{2(-1)}\big)\right] + 2n^2n^3\left[\mathrm{i}\sqrt{\frac{2\pi}{15}}\big(Y_{21} + Y_{2(-1)}\big)\right]\Bigg]$$

Sorting terms and making use of the fact that $\vec{n}$ is an unit vector, it remains

$$\begin{aligned} \ldots = |\vec{p}|^2\Bigg[&\frac{\sqrt{4\pi}}{3}Y_{00} + \sqrt{\frac{2}{3}}\big[3(n^3)^2 - 1\big]\sqrt{\frac{2\pi}{15}}Y_{20} \\ &+ (n^1 - \mathrm{i}n^2)^2\sqrt{\frac{2\pi}{15}}Y_{22} + (n^1 + \mathrm{i}n^2)^2\sqrt{\frac{2\pi}{15}}Y_{2(-2)} \\ &- 2(n^1 - \mathrm{i}n^2)n^3\sqrt{\frac{2\pi}{15}}Y_{21} + 2(n^1 + \mathrm{i}n^2)n^3\sqrt{\frac{2\pi}{15}}Y_{2(-1)}\Bigg] \end{aligned} \tag{5.23}$$

We thus end up with the following two non-vanishing multipole moments at second order in perturbation theory for Lorentz boosts

$$(\Delta^2)_{00}(p^0, |\vec{p}|) = \sqrt{\pi}\left[\varepsilon p^0 + \frac{1}{3}\varepsilon^2|\vec{p}|^2\right]\mathrm{e}^{\varepsilon p^0}\begin{pmatrix} p^0 \\ |\vec{p}| \\ 0 \\ 0 \\ \mu \end{pmatrix}$$

$$(\Delta^2)_{2m}(p^0, |\vec{p}|) = \sqrt{\frac{\pi}{30}}\varepsilon^2|\vec{p}|^2\mathrm{e}^{\varepsilon p^0}\begin{pmatrix} p^0 \\ |\vec{p}| \\ 0 \\ 0 \\ \mu \end{pmatrix} \times \begin{cases} \sqrt{\frac{2}{3}}\big[3(n^3)^2 - 1\big] & \text{for } m = 0 \\ \mp 2(n^1 \mp \mathrm{i}n^2)n^3 & \text{for } m = \pm 1 \\ (n^1 \pm \mathrm{i}n^2)^2 & \text{for } m = \pm 2 \end{cases}$$

This concludes the proof. □

[a]Note that due to our choice of the regularized kernel of the fermionic projector where $\widehat{v^{\varepsilon}_{\alpha}}(p) \propto p^{\alpha}$, only the radial spherical harmonics $\vec{Y}_{1m}$ appear while the tangential components proportional to $\vec{\Psi}_{1m}$ and $\vec{\Phi}_{1m}$ vanish identically. This is exactly the same as already explained in Lemma 5.1.2.

In order to apply Theorem 5.1.4 to this result, it remains to determine the corresponding functions $f^{(n)}_{lm}$ to establish the connection with Lemma 5.1.2.

Corollary 5.2.2 (Functions $f^{(n)}_{lm}$ for Lorentz Boosts)

In order to reproduce Lorentz boosts of the four-velocity in direction $\vec{n} \in \mathbb{R}^3$ as derived in Lemma 5.2.1, the functions $f^{(n)}_{lm}$ in Lemma 5.1.2 have to be chosen as

$$f^{(1)}_{1m}(p^0, |\vec{p}|) = \sqrt{\frac{4\pi}{3}}\frac{|\vec{p}|}{p^0}\begin{cases} n^3 & \text{for } m = 0 \\ \mp\frac{n^1 \mp \mathrm{i}n^2}{\sqrt{2}} & \text{for } m = \pm 1 \end{cases} \quad \text{and} \quad f^{(2)}_{00}(p^0, |\vec{p}|) = \sqrt{4\pi} \tag{5.24}$$

while all other functions $f^{(n)}_{lm}$ vanish identically.

Proof. To determine the functions $f_{lm}^{(n)}$ for Lorentz boosts, we proceed order by order in the perturbation index n and consider the different multipole orders l as substeps.

(1) Perturbation Order $n = 1$

As there exists no term at multipole order $l = 0$ in (5.17), we can immediately conclude that $f_{00}^{(1)}$ vanishes identically. At multipole order $l = 1$ we find by comparison of (5.17a) with (5.2a) that the functions $f_{1m}^{(1)}(|\vec{p}|)$ in Lemma 5.1.2 have to be chosen as

$$f_{1m}^{(1)}(p^0, |\vec{p}|) = \sqrt{\frac{4\pi}{3}}\frac{|\vec{p}|}{p^0}\begin{cases} n^3 & \text{for } m = 0 \\ \mp\frac{n^1 \mp i n^2}{\sqrt{2}} & \text{for } m = \pm 1 \end{cases} \tag{5.25}$$

in order to reproduce Lorentz boosts. For higher multipole orders $l \geq 2$ we can conclude that all functions $f_{lm}^{(1)}$ must vanish identically.

(2) Perturbation Order $n = 2$

As a consequence of the appearance of the functions $f_{lm}^{(1,1)}$ in (5.2b), the considerations at second order in perturbation theory are slightly more involved.

(a) Multipole Order $l = 0$

While there was no term for $l = 0$ at first perturbation order, for $n = 2$ we now have a term at multipole order $l = 0$. Comparing (5.17b) with (5.2b) order-by-order in ε leads to the requirements

$$\frac{f_{00}^{(2)}(p^0, |\vec{p}|)}{2} \stackrel{!}{=} \sqrt{\pi} \qquad \text{and} \qquad \frac{f_{00}^{(1,1)}(p^0, |\vec{p}|)}{2} \stackrel{!}{=} \frac{\sqrt{\pi}}{3}\left(\frac{|\vec{p}|}{p^0}\right)^2 \tag{5.26}$$

where, according to the definition of $f_{00}^{(1,1)}$ in (5.2b,i), the latter requirement must be understood merely as a consistency condition. Explicitly, we have

$$f_{00}^{(1,1)}(p^0, |\vec{p}|) \stackrel{(5.2b,i)}{=} \sum_{l_1,m_1}\sum_{l_2,m_2} f_{l_1 m_1}^{(1)}(p^0, |\vec{p}|) f_{l_2 m_2}^{(1)}(p^0, |\vec{p}|)\sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi}} \times \\ \times \begin{pmatrix} l_1 & l_2 & 0 \\ m_1 & m_2 & 0 \end{pmatrix}\begin{pmatrix} l_1 & l_2 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Taking into account that the functions $f_{lm}^{(1)}$ vanish identically except for $l = 1$, the expression reduces to

$$\ldots = \sum_{m_1,m_2=-1}^{1} f_{1m_1}^{(1)}(p^0, |\vec{p}|) f_{1m_2}^{(1)}(p^0, |\vec{p}|)\sqrt{\frac{9}{4\pi}}\begin{pmatrix} 1 & 1 & 0 \\ m_1 & m_2 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Evaluating the remaining Wigner $3j$ symbols where the first one vanishes except for $m_1 = -m_2$, we finally arrive at[78, p. 138]

$$f_{00}^{(1,1)}(p^0, |\vec{p}|) \stackrel{(5.25)}{=} \frac{\sqrt{4\pi}}{3}\left(\frac{|\vec{p}|}{p^0}\right)^2 |\vec{n}|^2 \tag{5.27}$$

which, since $\vec{n}$ is a unit vector, proves that the claimed condition is satisfied.

(b) Multipole Order $l = 1$

At multipole order $l = 1$ there is no term, i. e. $f_{1m}^{(2)} = 0$ for $m \in \{0, \pm 1\}$.

(c) Multipole Order $l = 2$

By analogy with the above considerations, we find two conditions at multipole order $l = 2$, namely

$$f^{(2)}_{2m}(p^0, |\vec{p}|) \overset{!}{=} 0 \quad \text{and} \quad \frac{f^{(1,1)}_{2m}(p^0, |\vec{p}|)}{2} \overset{!}{=} \sqrt{\frac{\pi}{30}} \left(\frac{|\vec{p}|}{p^0}\right)^2 \begin{cases} \sqrt{\frac{2}{3}}\Big[3(n^3)^2 - 1\Big] & \text{for } m = 0 \\ \mp 2(n^1 \mp \mathrm{i}n^2)n^3 & \text{for } m = \pm 1 \\ (n^1 \mp \mathrm{i}n^2)^2 & \text{for } m = \pm 2 \end{cases}$$

where the latter one is again a consistency condition. Taking into account that at perturbation order $n = 1$ the only non-vanishing functions are those with $l = 1$, the condition collapses to

$$f^{(1,1)}_{2m}(p^0, |\vec{p}|) \overset{!}{=} (-1)^m \sum_{m_1, m_2 = -1}^{1} \sqrt{\frac{45}{4\pi}} \begin{pmatrix} 1 & 1 & 2 \\ m_1 & m_2 & -m \end{pmatrix} \begin{pmatrix} 1 & 1 & 2 \\ 0 & 0 & 0 \end{pmatrix} f^{(1)}_{1m_1}(p^0, |\vec{p}|) f^{(1)}_{1m_2}(p^0, |\vec{p}|)$$

where the second Wigner $3j$ symbol evaluates to $\sqrt{\frac{2}{15}}$. Taking into account that the condition for the first Wigner $3j$ symbol to be non-vanishing is given by $m_1 + m_2 - m = 0$, we find for $m \in \{0, \pm 1, \pm 2\}$

$$\begin{aligned} f^{(1,1)}_{20}(p^0, |\vec{p}|) &\overset{!}{=} \sqrt{\frac{6}{4\pi}} \Bigg[2 \cdot \begin{pmatrix} 1 & 1 & 2 \\ 1 & -1 & 0 \end{pmatrix} f^{(1)}_{11}(p^0, |\vec{p}|) f^{(1)}_{1(-1)}(p^0, |\vec{p}|) \\ &\qquad + \begin{pmatrix} 1 & 1 & 2 \\ 0 & 0 & 0 \end{pmatrix} f^{(1)}_{10}(|\vec{p}|) f^{(1)}_{10}(|\vec{p}|) \Bigg] \\ &= \sqrt{\frac{8\pi}{3}} \left(\frac{|\vec{p}|}{p^0}\right)^2 \left[2 \cdot \sqrt{\frac{1}{30}} \left(-\frac{(n^1)^2 + (n^2)^2}{2} \right) + \sqrt{\frac{2}{15}} (n^3)^2 \right] \\ &= \sqrt{\frac{16\pi}{45}} \left(\frac{|\vec{p}|}{p^0}\right)^2 \left[-\frac{(n^1)^2 + (n^2)^2 + (n^3)^2 - (n^3)^2}{2} + (n^3)^2 \right] \\ &= \sqrt{\frac{4\pi}{45}} \left(\frac{|\vec{p}|}{p^0}\right)^2 \Big[-1 + 3(n^3)^2 \Big] \end{aligned}$$

$$\begin{aligned} f^{(1,1)}_{2(\pm 1)}(p^0, |\vec{p}|) &\overset{!}{=} (-2) \cdot \sqrt{\frac{6}{4\pi}} \begin{pmatrix} 1 & 1 & 2 \\ \pm 1 & 0 & \mp 1 \end{pmatrix} f^{(1)}_{1(\pm 1)}(p^0, |\vec{p}|) f^{(1)}_{10}(p^0, |\vec{p}|) \\ &= \sqrt{\frac{8\pi}{3}} \left(\frac{|\vec{p}|}{p^0}\right)^2 \cdot (-2) \cdot \left(-\sqrt{\frac{1}{10}} \right) \left(\mp \frac{n^1 \mp \mathrm{i}n^2}{\sqrt{2}} \right) n^3 \\ &= \sqrt{\frac{8\pi}{15}} \left(\frac{|\vec{p}|}{p^0}\right)^2 \Big[\mp (n^1 \mp \mathrm{i}n^2) n^3 \Big] \end{aligned}$$

$$\begin{aligned} f^{(1,1)}_{2(\pm 2)}(p^0, |\vec{p}|) &\overset{!}{=} \sqrt{\frac{6}{4\pi}} \begin{pmatrix} 1 & 1 & 2 \\ \pm 1 & \pm 1 & \mp 2 \end{pmatrix} f^{(1)}_{1(\pm 1)}(p^0, |\vec{p}|) f^{(1)}_{1(\pm 1)}(p^0, |\vec{p}|) \\ &= \sqrt{\frac{8\pi}{3}} \left(\frac{|\vec{p}|}{p^0}\right)^2 \sqrt{\frac{1}{5}} \left(\mp \frac{n^1 \mp \mathrm{i}n^2}{\sqrt{2}} \right)^2 \\ &= \sqrt{\frac{2\pi}{15}} \left(\frac{|\vec{p}|}{p^0}\right)^2 (n^1 \mp \mathrm{i}n^2)^2 \end{aligned}$$

which concludes the proof that the conditions at multipole order $l = 2$ are satisfied.

(d) Multipole Order $l \geq 3$

At multipole order $l \geq 3$ there are no terms, i. e. $f^{(2)}_{lm} = 0$ for all $l \geq 3$.

(3) Conclusion

To summarize, we find that Lorentz boosts as derived in Lemma 5.2.1 can be reproduced from (5.2) by choosing the functions $f_{lm}^{(n)}$ as

$$f_{1m}^{(1)}(p^0,|\vec{p}|) = \sqrt{\frac{4\pi}{3}}\frac{|\vec{p}|}{p^0}\begin{cases} n^3 & \text{for } m=0 \\ \mp\frac{n^1\mp in^2}{\sqrt{2}} & \text{for } m=\pm 1\end{cases} \qquad \text{and} \qquad f_{00}^{(2)}(p^0,|\vec{p}|) = \sqrt{4\pi}$$

while all other functions vanish identically.

This concludes the proof. □

5.2.2 Variation of the Regularized Causal Action for Lorentz Boosts

After the preparatory calculations in the previous section, we now combine the results from Corollary 5.2.2 and Theorem 5.1.4 to evaluate the variation of the regularized causal action for Lorentz boosts of the four-velocity of the regularization.

Lemma 5.2.3 (Variation of the Regularized Causal Action for Lorentz Boosts)

The variation of the regularized causal action as given in Theorem 5.1.4 evaluates for Lorentz boosts of the four-velocity of the regularization to

$$\delta\mathcal{S}^\varepsilon = 0 \tag{5.28a}$$

$$\delta^2\mathcal{S}^\varepsilon = \mathrm{Re}\left[\int_0^\infty \mathrm{d}|\vec{p}|\ \left(\sqrt{\pi}Q_0^\varepsilon(|\vec{p}|) + \int_0^\infty \mathrm{d}|\vec{q}|\ \frac{2\pi}{3}\frac{|\vec{p}||\vec{q}|Q_{10}^\varepsilon(|\vec{p}|,|\vec{q}|)}{\omega_p\omega_q}\right)\right] \tag{5.28b}$$

Proof. In order to evaluate the expression for the variation of the regularized causal action as derived in Theorem 5.1.4, we consider the contributions at first and second perturbation order separately.

(1) Evaluation of $\delta\mathcal{S}^\varepsilon$ for Lorentz Boosts

According to (5.13a), the first variation of the regularized causal action only depends on the function $f_{00}^{(1)}$ which vanishes identically in the case of Lorentz boosts. We thus immediately conclude that the first variation of the regularized causal action vanishes

$$\delta\mathcal{S}^\varepsilon\left[\left(f_{00}^{(1)}\right)^{\mathrm{LB}}\right] = 0$$

which means that Lorentz boosts are candidates for stationary points of $\mathcal{S}^\varepsilon$.

(2) Evaluation of $\delta^2\mathcal{S}^\varepsilon$ for Lorentz Boosts

Evaluating (5.13b) for Lorentz boosts by inserting (5.24) and taking into account that the scalar-valued integral kernels Q_{lm}^ε from (5.13b,i) satisfy the relation $Q_{1(\pm1)}^\varepsilon = Q_{10}^\varepsilon$, we find

$$\begin{aligned}\delta^2\mathcal{S}^\varepsilon\left[\left(f_{1m}^{(1)}\right)^{\mathrm{LB}},\left(f_{00}^{(2)}\right)^{\mathrm{LB}}\right] = \\ \overset{(5.13b)}{=} \mathrm{Re}\Bigg[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\ \Bigg(\frac{Q_0^\varepsilon(|\vec{p}|)}{2}f_{00}^{(2)}(|\vec{p}|) \\ +\frac{1}{2}\sum_{m=-1}^{1}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\ f_{1m}^{(1)}(|\vec{p}|)Q_{1m}^\varepsilon(|\vec{p}|,|\vec{q}|)\overline{f_{1m}^{(1)}(|\vec{q}|)}\Bigg)\Bigg]\end{aligned}$$

$$\overset{(5.24)}{=} \operatorname{Re}\left[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\left(\sqrt{\pi}Q_0^\varepsilon(|\vec{p}|) + \frac{1}{2}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\,\frac{4\pi}{3}Q_{10}^\varepsilon(|\vec{p}|,|\vec{q}|)\times\right.\right.$$
$$\left.\left.\times\frac{|\vec{p}||\vec{q}|}{\omega_p\omega_q}\left[(n^3)^2 + \left|\frac{n^1 - \mathrm{i}n^2}{\sqrt{2}}\right|^2 + \left|\frac{n^1 + \mathrm{i}n^2}{\sqrt{2}}\right|^2\right]\right)\right]$$
$$\overset{(5.24)}{=} \operatorname{Re}\left[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\left(\sqrt{\pi}Q_0^\varepsilon(|\vec{p}|) + \int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\,\frac{2\pi}{3}\,\frac{|\vec{p}||\vec{q}|Q_{10}^\varepsilon(|\vec{p}|,|\vec{q}|)}{\omega_p\omega_q}\right)\right]$$

where in the last step we used that $\vec{n}$ has unit length. This concludes the proof. □

According to this lemma, Lorentz boosts are candidates for stationary points of the regularized causal action. To show that Lorentz boosts actually leave $\mathcal{S}^\varepsilon$ invariant (at least up to second order in perturbation theory), it remains to show that the second variation of the regularized causal action as computed in (5.28b) vanishes. To this end, we need the following lemma.

Lemma 5.2.4 (Condition on Derivatives of the Regularized Causal Lagrangian)

The iε-regularized causal Lagrangian as given in (2.42) satisfies the condition

$$0 = \int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0, r)\,\left[\frac{r^4}{3}D^2\mathcal{L}^\varepsilon(\xi) + \xi^0 r^2 D\mathcal{L}^\varepsilon(\xi)\right] - \int_{\mathbb{R}} \mathrm{d}\xi^0\,\left[\frac{r^4}{3}\frac{\left(D\mathcal{L}^\varepsilon(\xi)\right)^2}{\partial_r\mathcal{L}^\varepsilon(\xi)}\right]\Bigg|_{r=R^\varepsilon_{\max}(\xi^0)} \tag{5.29}$$

where D denotes the differential operator with respect to ξ^0 and r given by $D = \partial_{\xi^0} + \frac{\xi^0}{r}\partial_r$.

Proof. In order to prove the claimed relation, we will repeatedly make use of the following two equivalent ways to express the integral over the region $\mathfrak{X}^\varepsilon$

$$\int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0, r)\; f(\xi^0, r) = \int_0^\infty \mathrm{d}r\left(\int_{-\infty}^{-T^\varepsilon_{\min}(r)} \mathrm{d}\xi^0 + \int_{T^\varepsilon_{\min}(r)}^\infty \mathrm{d}\xi^0\right) f(\xi^0, r) \tag{5.30a}$$

$$\int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0, r)\; f(\xi^0, r) = \int_{\mathbb{R}} \mathrm{d}\xi^0 \int_0^{R^\varepsilon_{\max}(\xi^0)} \mathrm{d}r\; f(\xi^0, r) \tag{5.30b}$$

which we refer to as the $T^\varepsilon_{\min}$-representation and the $R^\varepsilon_{\max}$-representation of the bulk integral, respectively. Here the function $T^\varepsilon_{\min} : \mathbb{R}^+_0 \to \mathbb{R}^+_0$ is defined as

$$T^\varepsilon_{\min}(r) = \begin{cases} 0 & \text{for } 0 \le r \le R^\varepsilon_{\max}(0) \\ (R^\varepsilon_{\max})^{-1}(r) & \text{for } r > R^\varepsilon_{\max}(0) \end{cases} \tag{5.31}$$

(1) Evaluation of the Bulk Term

We start by considering the first term in the expression, referred to as the bulk term. Splitting up the outer differential operator D leads to

$$\int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0, r)\,\left[\frac{r^4}{3}\left(\frac{\partial}{\partial\xi^0} + \frac{\xi^0}{r}\frac{\partial}{\partial r}\right)D\mathcal{L}^\varepsilon(\xi) + \xi^0 r^2 D\mathcal{L}^\varepsilon(\xi)\right]$$
$$= \int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0, r)\,\left[\frac{r^4}{3}\frac{\partial}{\partial\xi^0}D\mathcal{L}^\varepsilon(\xi) + \frac{\xi^0 r^3}{3}\frac{\partial}{\partial r}D\mathcal{L}^\varepsilon(\xi) + \xi^0 r^2 D\mathcal{L}^\varepsilon(\xi)\right]$$

Making use of the $T^\varepsilon_{\min}$-representation from (5.30a) to integrate by parts with respect to ξ^0 in the first term we arrive at

$$\ldots \overset{(5.30a)}{=} \int_0^\infty \mathrm{d}r\ \frac{r^4}{3}\left(\int_{-\infty}^{-T^\varepsilon_{\min}(r)} \mathrm{d}\xi^0\ \frac{\partial D\mathcal{L}^\varepsilon}{\partial \xi^0} + \int_{T^\varepsilon_{\min}(r)}^{\infty} \mathrm{d}\xi^0\ \frac{\partial D\mathcal{L}^\varepsilon}{\partial \xi^0}\right) + \int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0, r)\ \frac{\partial}{\partial r}\left[\frac{\xi^0 r^3}{3} D\mathcal{L}^\varepsilon(\xi)\right]$$

$$= \int_0^\infty \mathrm{d}r\ \frac{r^4}{3}\left(\Big[D\mathcal{L}^\varepsilon(\xi)\Big]_{-\infty}^{-T^\varepsilon_{\min}(r)} + \Big[D\mathcal{L}^\varepsilon(\xi)\Big]_{T^\varepsilon_{\min}(r)}^{\infty}\right) + \int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0, r)\ \frac{\partial}{\partial r}\left[\frac{\xi^0 r^3}{3} D\mathcal{L}^\varepsilon(\xi)\right]$$

where we have combined the second and third term into a partial derivative with respect to r along the way. The integrand of the first term can be simplified by observing that derivatives of $\mathcal{L}^\varepsilon(\xi)$ both with respect to ξ^0 and r vanish in the limit $\xi^0 \to \pm\infty$. This can be easily seen from an asymptotic expansion of derivatives of the modified Bessel functions of the second kind contained in (2.42).[57, 8.451/6] Thus, it remains

$$\cdots = \int_0^\infty \mathrm{d}r\ \frac{r^4}{3}\Big[D\mathcal{L}^\varepsilon(\xi)\Big]_{T^\varepsilon_{\min}(r)}^{-T^\varepsilon_{\min}(r)} + \int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0, r)\ \frac{\partial}{\partial r}\left[\frac{\xi^0 r^3}{3} D\mathcal{L}^\varepsilon(\xi)\right]$$

In this expression the second integral can also be simplified: Making use of the $R^\varepsilon_{\max}$-representation of the bulk integral from (5.30b) and taking into account that $D\mathcal{L}^\varepsilon(\xi)$ yields a finite value for $r = 0$ such that $r^3\mathcal{L}^\varepsilon(\xi)$ vanishes in the limit $r \to 0$, we end up with

$$\int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0, r)\ \left[\frac{r^4}{3}\left(\frac{\partial}{\partial \xi^0} + \frac{\xi^0}{r}\frac{\partial}{\partial r}\right) D\mathcal{L}^\varepsilon(\xi) + \xi^0 r^2 D\mathcal{L}^\varepsilon(\xi)\right]$$

$$\overset{(5.30b)}{=} - \int_0^\infty \mathrm{d}r\ \frac{r^4}{3}\Big[D\mathcal{L}^\varepsilon(\xi)\Big]_{-T^\varepsilon_{\min}(r)}^{T^\varepsilon_{\min}(r)} + \int_{\mathbb{R}} \mathrm{d}\xi^0\ \left[\frac{\xi^0 r^3}{3} D\mathcal{L}^\varepsilon(\xi)\right]\bigg|_{r=R^\varepsilon_{\max}(\xi^0)}$$

for the bulk term.

(2) Evaluation of the Boundary Term

Having simplified the bulk term, we now turn to the boundary term of the original expression. Combining the factor $\big(\partial_r \mathcal{L}^\varepsilon(\xi)\big)^{-1}$ with one of the factors $D\mathcal{L}^\varepsilon(\xi)$ yields

$$- \int_{\mathbb{R}} \mathrm{d}\xi^0\ \left[\frac{r^4}{3}\frac{1}{\partial_r \mathcal{L}^\varepsilon(\xi)}\big(D\mathcal{L}^\varepsilon(\xi)\big)^2\right]\bigg|_{r=R^\varepsilon_{\max}(\xi^0)} =$$

$$= - \int_{\mathbb{R}} \mathrm{d}\xi^0\ \left[\frac{r^4}{3}\frac{1}{\partial_r \mathcal{L}^\varepsilon(\xi)}\left(\frac{\partial \mathcal{L}^\varepsilon(\xi)}{\partial \xi^0} + \frac{\xi^0}{r}\frac{\partial \mathcal{L}^\varepsilon(\xi)}{\partial r}\right) D\mathcal{L}^\varepsilon(\xi)\right]\bigg|_{r=R^\varepsilon_{\max}(\xi^0)}$$

$$= - \int_{\mathbb{R}} \mathrm{d}\xi^0\ \left[\frac{r^4}{3}\left(\frac{\partial_{\xi^0} \mathcal{L}^\varepsilon(\xi)}{\partial_r \mathcal{L}^\varepsilon(\xi)} + \frac{\xi^0}{r}\right) D\mathcal{L}^\varepsilon(\xi)\right]\bigg|_{r=R^\varepsilon_{\max}(\xi^0)}$$

To proceed, we exploit the fact that the regularized causal Lagrangian by definition vanishes at the boundary $r = R^\varepsilon_{\max}(\xi^0)$. By differentiating this relation with respect to ξ^0 we obtain

$$0 = \frac{\mathrm{d}}{\mathrm{d}\xi^0}\Big(\mathcal{L}^\varepsilon(\xi)\big|_{r=R^\varepsilon_{\max}(\xi^0)}\Big) = \frac{\partial \mathcal{L}^\varepsilon(\xi)}{\partial \xi^0}\bigg|_{r=R^\varepsilon_{\max}(\xi^0)} + \frac{\partial \mathcal{L}^\varepsilon(\xi)}{\partial r}\bigg|_{r=R^\varepsilon_{\max}(\xi^0)} \frac{\mathrm{d}R^\varepsilon_{\max}(\xi^0)}{\mathrm{d}\xi^0}$$

Solving for the derivative of $\mathcal{L}^\varepsilon(\xi)$ with respect to ξ^0 and inserting the result into the previous expression results in

$$- \int_{\mathbb{R}} \mathrm{d}\xi^0\ \left[\frac{r^4}{3}\frac{1}{\partial_r \mathcal{L}^\varepsilon(\xi)}\big(D\mathcal{L}^\varepsilon(\xi)\big)^2\right]\bigg|_{r=R^\varepsilon_{\max}(\xi^0)} =$$

$$= -\int_{\mathbb{R}} \mathrm{d}\xi^0 \left[\left(-\frac{r^4}{3} \frac{\mathrm{d}R^\varepsilon_{\max}(\xi^0)}{\mathrm{d}\xi^0} + \frac{\xi^0 r^3}{3} \right) D\mathcal{L}^\varepsilon(\xi) \right] \Big|_{r=R^\varepsilon_{\max}(\xi^0)}$$

for the boundary term.

(3) Combining Bulk and Boundary Terms
Adding up the bulk and boundary contributions and cancelling terms we arrive at

$$\int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0, r) \left[\frac{r^4}{3} D^2\mathcal{L}^\varepsilon(\xi) + \xi^0 r^2 D\mathcal{L}^\varepsilon(\xi) \right] - \int_{\mathbb{R}} \mathrm{d}\xi^0 \left[\frac{r^4}{3} \frac{1}{\partial_r \mathcal{L}^\varepsilon(\xi)} \big(D\mathcal{L}^\varepsilon(\xi)\big)^2 \right] \Big|_{r=R^\varepsilon_{\max}(\xi^0)}$$
$$= -\int_0^\infty \mathrm{d}r \; \frac{r^4}{3} \Big[D\mathcal{L}^\varepsilon(\xi) \Big]_{-T^\varepsilon_{\min}(r)}^{T^\varepsilon_{\min}(r)} + \int_{\mathbb{R}} \mathrm{d}\xi^0 \; \frac{\mathrm{d}R^\varepsilon_{\max}(\xi^0)}{\mathrm{d}\xi^0} \left[\frac{r^4}{3} D\mathcal{L}^\varepsilon(\xi) \right] \Big|_{r=R^\varepsilon_{\max}(\xi^0)}$$

To demonstrate that this expression vanishes, we split the domain of integration in the second term into regions where $\xi^0 < 0$ and $\xi^0 > 0$, respectively. As a consequence of this splitting, we can express ξ^0 as $\xi^0 = -T^\varepsilon_{\min}(R^\varepsilon_{\max}(\xi^0))$ and $\xi^0 = T^\varepsilon_{\min}(R^\varepsilon_{\max}(\xi^0))$, respectively, and thus obtain

$$\cdots = -\int_0^\infty \mathrm{d}r \; \frac{r^4}{3} D\mathcal{L}^\varepsilon\big(T^\varepsilon_{\min}(r), r\big) + \int_0^\infty \mathrm{d}\xi^0 \; \frac{\mathrm{d}R^\varepsilon_{\max}(\xi^0)}{\mathrm{d}\xi^0} \left[\frac{r^4}{3} D\mathcal{L}^\varepsilon\big(T^\varepsilon_{\min}(r), r\big) \right] \Big|_{r=R^\varepsilon_{\max}(\xi^0)}$$
$$+ \int_0^\infty \mathrm{d}r \; \frac{r^4}{3} D\mathcal{L}^\varepsilon\big(-T^\varepsilon_{\min}(r), r\big) + \int_{-\infty}^0 \mathrm{d}\xi^0 \; \frac{\mathrm{d}R^\varepsilon_{\max}(\xi^0)}{\mathrm{d}\xi^0} \left[\frac{r^4}{3} D\mathcal{L}^\varepsilon\big(-T^\varepsilon_{\min}(r), r\big) \right] \Big|_{r=R^\varepsilon_{\max}(\xi^0)}$$

Splitting the integrals in the first and third term and changing variables in the second and fourth term gives

$$\cdots = -\left(\int_0^{R^\varepsilon_{\max}(0)} \mathrm{d}r + \int_{R^\varepsilon_{\max}(0)}^\infty \mathrm{d}r \right) \frac{r^4}{3} D\mathcal{L}^\varepsilon\big(T^\varepsilon_{\min}(r), r\big) + \lim_{\tau\to\infty} \int_{R^\varepsilon_{\max}(0)}^{R^\varepsilon_{\max}(\tau)} \mathrm{d}u \; \frac{u^4}{3} D\mathcal{L}^\varepsilon\big(T^\varepsilon_{\min}(u), u\big)$$
$$+ \left(\int_0^{R^\varepsilon_{\max}(0)} \mathrm{d}r + \int_{R^\varepsilon_{\max}(0)}^\infty \mathrm{d}r \right) \frac{r^4}{3} D\mathcal{L}^\varepsilon\big(-T^\varepsilon_{\min}(r), r\big) + \lim_{\tau\to\infty} \int_{R^\varepsilon_{\max}(-\tau)}^{R^\varepsilon_{\max}(0)} \mathrm{d}u \; \frac{u^4}{3} D\mathcal{L}^\varepsilon\big(-T^\varepsilon_{\min}(u), u\big)$$

Recalling that the function $R^\varepsilon_{\max}$ satisfies $\lim_{\tau\to\infty} R^\varepsilon_{\max}(\pm\tau) = \infty$, we realize that the second and third term in the first line both describe the integral over the same set $\mathfrak{C}^\varepsilon_+ = \{(\xi^0, r) \,|\, \xi^0 \geq 0, r = R^\varepsilon_{\max}(\xi^0)\}$, namely the upper regularized light-cone, and thus add up to zero. Likewise, the two terms in the second line cancel as they both describe the integral over the same set $\mathfrak{C}^\varepsilon_- = \{(\xi^0, r) \,|\, \xi^0 \leq 0, r = R^\varepsilon_{\max}(\xi^0)\}$ being the lower regularized light-cone. We thus end up with

$$\int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0, r) \left[\frac{r^4}{3} D^2\mathcal{L}^\varepsilon(\xi) + \xi^0 r^2 D\mathcal{L}^\varepsilon(\xi) \right] - \int_{\mathbb{R}} \mathrm{d}\xi^0 \left[\frac{r^4}{3} \frac{1}{\partial_r \mathcal{L}^\varepsilon(\xi)} \big(D\mathcal{L}^\varepsilon(\xi)\big)^2 \right] \Big|_{r=R^\varepsilon_{\max}(\xi^0)}$$
$$= -\int_0^{R^\varepsilon_{\max}(0)} \mathrm{d}r \; \frac{r^4}{3} D\mathcal{L}^\varepsilon\big(T^\varepsilon_{\min}(r), r\big) + \int_0^{R^\varepsilon_{\max}(0)} \mathrm{d}r \; \frac{r^4}{3} D\mathcal{L}^\varepsilon\big(-T^\varepsilon_{\min}(r), r\big) \tag{5.32}$$

But since $T^\varepsilon_{\min}(r)$ vanishes for $0 \leq r \leq R^\varepsilon_{\max}(0)$ according to (5.31), both terms add up to zero such that the whole expression vanishes.

This concludes the proof. □

This lemma is the crucial ingredient in proving that the second variation of the regularized causal action vanishes for Lorentz boosts of the velocity vector of the regularization. The missing link which establishes the connection between Lemma 5.2.3 and Lemma 5.2.4 is to show that the second variation as derived in (5.28b) is the same as the left-hand side in (5.29). Since this is a rather technical task, we have deferred this to Appendix F and here in particular Lemma F.2.2. Combining these results, we can now formulate the following theorem.

Theorem 5.2.5 (Invariance of $\mathcal{S}^\varepsilon$ under Lorentz Boosts)

The iε-regularized causal action $\mathcal{S}^\varepsilon$ is invariant under Lorentz boosts of the velocity vector of the regularization.

Proof. In Lemma 5.2.3 we have shown that Lorentz boosts are at least stationary points of the iε-regularized causal action as $\delta\mathcal{S}^\varepsilon$ vanishes, while the expression for $\delta^2\mathcal{S}^\varepsilon$ reads

$$\delta^2\mathcal{S}^\varepsilon \overset{(5.28b)}{=} \mathrm{Re}\left[\int_0^\infty \mathrm{d}|\vec{p}|\,\left(\sqrt{\pi}Q_0^\varepsilon(|\vec{p}|) + \int_0^\infty \mathrm{d}|\vec{q}|\,\frac{2\pi}{3}\frac{|\vec{p}||\vec{q}|Q_{10}^\varepsilon(|\vec{p}|,|\vec{q}|)}{\omega_p\omega_q}\right)\right]$$

Making use of Lemma F.2.2, this expression evaluates to

$$\delta^2\mathcal{S}^\varepsilon \overset{(F.7)}{=} 2\pi\left[\int_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0,r)\,\left(\xi^0 r^2 D\mathcal{L}^\varepsilon(\xi) + \frac{r^4}{3}D^2\mathcal{L}^\varepsilon(\xi)\right) - \int_{\mathbb{R}} \mathrm{d}\xi^0\,\frac{r^4}{3}\frac{\left(D\mathcal{L}^\varepsilon(\xi)\right)^2}{\partial_r\mathcal{L}^\varepsilon(\xi)}\bigg|_{r=R^\varepsilon_{\max}(\xi^0)}\right] \overset{(5.29)}{=} 0$$

which, according to Lemma 5.2.4, vanishes identically. Thus, Lorentz boosts of the velocity vector of the regularization are not only stationary points of the iε-regularized causal action, but they leave the causal action invariant. □

Having studied special variations of the regularized kernel of the fermionic projector corresponding to Lorentz boosts of the velocity vector of the regularization, we now come back to the more general variations from Lemma 5.1.2 and examine how the regularized causal action reacts on initial perturbations via the causal action principle.

5.3 Perturbations and Compensations

The starting point of our considerations is a spherically-symmetrically iε-regularized kernel of the fermionic projector $\widehat{\mathrm{P}_0^\varepsilon}$, which is assumed to be a minimizer of the regularized causal action. This regularized kernel of the fermionic projector corresponds to a regularized Dirac sea configuration in Minkowski spacetime equipped with a certain spherically-symmetric microstructure. Now, if this spherically-symmetric situation is destroyed by some slight deformation of the microstructure, also the regularized kernel of the fermionic projector changes. For reasons of manageability we assume that the deformation only affects the exponential factor $\mathrm{e}^{\varepsilon|p^0|}$ in the sense that it is replaced by an anisotropic equivalent as defined in Assumption 5.1.1. The resulting anisotropically iε-regularized kernel of the fermionic projector $\widehat{\mathrm{P}_\tau^\varepsilon}$ is no longer a minimizer of the regularized causal action. According to the causal action principle, this non-optimal configuration causes a dynamics aimed at restoring a potentially new configuration which again extremizes the regularized causal action. In what follows, we give a simple model where an initial perturbation of the spherically symmetric iε-regularization is counterbalanced by so-called *compensations*.

5.3.1 Derivation of Compensations

On a technical level, we model the situation described above as follows: We assume that the anisotropically iε-regularized kernel of the fermionic projector in momentum space takes the for

$$\widehat{\mathrm{P}^\varepsilon_\tau}(p) = \big(\not{p} + \mu \mathrm{id}_{\mathbb{C}^4}\big)\delta(p^2-\mu^2)\Theta(-p^0)\mathrm{e}^{\varepsilon p^0 \varpi_\tau(p)} \tag{5.33a}$$

where, according to Assumption 5.1.1, $\varpi_\tau(p)$ is given by

$$\varpi_\tau(p) = 1 + \sum_{n=1}^{\infty}\sum_{l,m} \varpi^{(n)}_{lm}(p^0, |\vec{p}|) Y_{lm}(\theta_p, \varphi_p) \tag{5.33b}$$

For vanishing perturbation, namely in the limit $\tau \to 0$, the perturbed regularized kernel of the fermionic projector $\widehat{\mathrm{P}^\varepsilon_\tau}(p)$ reduces to $\widehat{\mathrm{P}^\varepsilon_0}(p) = \widehat{\mathrm{P}^\varepsilon}(p)$. Due to the fact that $\widehat{\mathrm{P}^\varepsilon_\tau}(p)$ does in general no longer extremalize the regularized causal action, the causal action principle tries to resolve this dissatisfying situation by further modifying the anisotropic iε-regularization through a so-called *compensation*. Once again, we assume for better manageability that the resulting regularized kernel of the fermionic projector still has the structure as given in Assumption 5.1.1.

Lemma 5.3.1 (Stationarity Condition for the Compensation)

Let $\widehat{\mathrm{P}^\varepsilon_\tau}(p)$ be the compensated regularized kernel of the fermionic projector given by

$$\widehat{\mathrm{P}^\varepsilon_\tau}(p) = \big(\not{p} + \mu \mathrm{id}_{\mathbb{C}^4}\big)\delta(p^2-\mu^2)\Theta(-p^0)\mathrm{e}^{\varepsilon p^0 [\varpi_\tau(p)+\kappa_\tau(p)]} \tag{5.34}$$

where

$$\varpi_\tau(p) = 1 + \sum_{n=1}^{\infty}\frac{\tau^n}{n!}\sum_{l,m} \varpi^{(n)}_{lm}(p^0, |\vec{p}|) Y_{lm}(\theta_p, \varphi_p) \tag{5.34a}$$

represents the anisotropic iε-regularization induced by the initial perturbation, while

$$\kappa_\tau(p) = \sum_{n=1}^{\infty}\frac{\tau^n}{n!}\sum_{l,m} \kappa^{(n)}_{lm}(p^0, |\vec{p}|) Y_{lm}(\theta_p, \varphi_p) \tag{5.34b}$$

stands for the compensation. Then $\widehat{\mathrm{P}^\varepsilon_\tau}(p)$ is a stationary point of the regularized causal action, if the multipole moments of the perturbation and the compensation satisfy the following condition

$$\begin{aligned}
&\forall (l,m) \in \mathbb{N}_0 \times \mathbb{Z} \text{ with } -l \le m \le l \;\forall f^{(1)}_{lm} \in C^\infty(\mathbb{R}^+_0, \mathbb{C}) : \\
&\mathrm{Re}\left[\sum_{l,m}\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\; \kappa^{(1)}_{lm}(|\vec{p}|) Q^\varepsilon_{lm}(|\vec{p}|,|\vec{q}|)\overline{f^{(1)}_{lm}(|\vec{q}|)}\right] \\
&\quad \overset{!}{=} -\mathrm{Re}\left[\sum_{l,m}\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\; \varpi^{(1)}_{lm}(|\vec{p}|) Q^\varepsilon_{lm}(|\vec{p}|,|\vec{q}|)\overline{f^{(1)}_{lm}(|\vec{q}|)}\right]
\end{aligned} \tag{5.35}$$

Proof. To prove the claimed relations, we recall that the first variation of the regularized causal action has two dependences: On the one hand it is a functional of $\widehat{\mathrm{P}^\varepsilon}$ while on the other hand it also depends on the first variation $\delta\widehat{\mathrm{P}^\varepsilon}$ around $\widehat{\mathrm{P}^\varepsilon}$. Therefore, the condition for $\widehat{\mathrm{P}^\varepsilon}$ to be a stationary point of the regularized causal action reads

$$\forall \delta\widehat{\mathrm{P}^\varepsilon_{\text{test}}} \in \mathcal{D}'(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4,\mathbb{C}^4)) : \qquad 0 \overset{!}{=} \left(\delta\mathcal{S}^\varepsilon\left[\widehat{\mathrm{P}^\varepsilon}\right]\right)\left[\delta\widehat{\mathrm{P}^\varepsilon_{\text{test}}}\right] \tag{5.36}$$

Based on this condition, we can now derive a relation between the initial perturbation and the resulting compensation: Choosing $\widehat{\mathrm{P}^\varepsilon}$ as the regularized kernel of the fermionic projector given by

$$\widehat{\mathrm{P}^\varepsilon_\tau}(p) = \big(\not{p} + \mu \mathrm{id}_{\mathbb{C}^4}\big)\delta(p^2-\mu^2)\Theta(-p^0)\mathrm{e}^{\varepsilon p^0(\varpi_\tau+\kappa_\tau)} \tag{5.37}$$

where ϖ_τ and κ_τ correspond to the initial perturbation and the resulting compensation, respectively, the condition for the compensated regularized kernel of the fermionic projector $\widehat{\mathrm{P}^\varepsilon_\tau}$ to be a stationary point of the regularized causal action reads

$$\forall \delta\widehat{\mathrm{P}^\varepsilon_{\text{test}}} \in \mathcal{D}'(\mathbb{R}^4, \mathrm{L}(\mathbb{C}^4,\mathbb{C}^4)): \quad 0 \stackrel{!}{=} \left(\delta\mathcal{S}^\varepsilon\left[\widehat{\mathrm{P}^\varepsilon_\tau}\right]\right)\left[\delta\widehat{\mathrm{P}^\varepsilon_{\text{test}}}\right]$$

Expanding this condition into a Taylor series up to second order in the parameter τ yields[a]

$$0 \stackrel{!}{=} \left(\delta\mathcal{S}^\varepsilon\left[\widehat{\mathrm{P}^\varepsilon_0}\right]\right)\left[\delta\widehat{\mathrm{P}^\varepsilon_{\text{test}}}\right] + \tau\left(\delta^2\mathcal{S}^\varepsilon_{\text{sql}}\left[\widehat{\mathrm{P}^\varepsilon_0}\right]\right)\left[\delta\widehat{\mathrm{P}^\varepsilon_{\text{pert}}} + \delta\widehat{\mathrm{P}^\varepsilon_{\text{comp}}}, \delta\widehat{\mathrm{P}^\varepsilon_{\text{test}}}\right] + \mathcal{O}(\tau^2)$$

Since $\widehat{\mathrm{P}^\varepsilon_0}$ is assumed to be a stationary point of the regularized causal action, the first term vanishes such that only the sesquilinear term remains. If we furthermore exploit sesquilinearity (see (4.53)), we arrive at the condition

$$\left(\delta^2\mathcal{S}^\varepsilon_{\text{sql}}\left[\widehat{\mathrm{P}^\varepsilon_0}\right]\right)\left[\delta\widehat{\mathrm{P}^\varepsilon_{\text{comp}}}, \delta\widehat{\mathrm{P}^\varepsilon_{\text{test}}}\right] \stackrel{!}{=} -\left(\delta^2\mathcal{S}^\varepsilon_{\text{sql}}\left[\widehat{\mathrm{P}^\varepsilon_0}\right]\right)\left[\delta\widehat{\mathrm{P}^\varepsilon_{\text{pert}}}, \delta\widehat{\mathrm{P}^\varepsilon_{\text{test}}}\right] \tag{5.38}$$

To arrive at the claimed expression, we now make use of the explicit expression for the sesquilinear term in the second variation of the regularized causal action as given in (5.13b). Denoting the multipole moments corresponding to the test variation by $f^{(n)}_{lm}$, we find the following condition which relates the multipole moments $\kappa^{(1)}_{lm}$ and $\varpi^{(1)}_{lm}$

$$\begin{aligned}
&\forall (l,m) \in \mathbb{N}_0 \times \mathbb{Z} \text{ with } -l \le m \le l \ \forall f^{(1)}_{lm} \in C^\infty(\mathbb{R}^+_0, \mathbb{C}):\\
&\mathrm{Re}\left[\sum_{l,m}\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\ \kappa^{(1)}_{lm}(|\vec{p}|)Q^\varepsilon_{lm}(|\vec{p}|,|\vec{q}|)\overline{f^{(1)}_{lm}(|\vec{q}|)}\right]\\
&\quad \stackrel{!}{=} -\mathrm{Re}\left[\sum_{l,m}\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\ \varpi^{(1)}_{lm}(|\vec{p}|)Q^\varepsilon_{lm}(|\vec{p}|,|\vec{q}|)\overline{f^{(1)}_{lm}(|\vec{q}|)}\right]
\end{aligned} \tag{5.39}$$

This concludes the proof. □

[a] Note that the second variation of the regularized causal action contains two terms, namely the term which depends linearly on the second variation of the regularized kernel of the fermionic projector and the sesquilinear term where the first variation of the regularized kernel of the fermionic projector enters twice. Due to the fact that in the present case the argument of the first variation is fixed already, we only obtain the sesquilinear term.

5.3.2 Variation of the Local Particle Density

To conclude this chapter, we finally want to analyze whether deformations of the regularization have an effect on the local particle density and, if so, quantify its strength. As explained in Chapter 2, the regularized kernel of the fermionic projector represents a certain Dirac sea configuration which, in Minkowski spacetime, is the entirety of negative-frequency solutions of the Dirac equation. As already mentioned in Footnote 9 on page 22, to every solution ψ of the Dirac equation one can associate the so-called *Dirac current* which is a four-vector field defined as

$$j^k(x) := \prec\psi|\gamma^k\psi\succ_{S_x} \tag{5.40}$$

with γ^k denoting the k^{th} Dirac matrix. The zeroth component $j^0(x)$ of this Dirac current can be interpreted as the *probability density* of the fermionic particle corresponding to the Dirac solution

ψ to be at the spacetime point $x \in \mathscr{M}$.[1] If one now considers not only one solution of the Dirac equation, but the entirety of all negative-frequency solutions described by the (regularized) kernel of the fermionic projector, the probability density generalizes to the concept of the *local particle density*.[2]

Definition 5.3.2 (Local Particle Density)

For a given homogeneous regularized kernel of the fermionic projector, the *local particle density* f is defined as[6, p. 68]

$$f := \operatorname{Tr}\left(\gamma^0 \mathrm{P}^\varepsilon(0)\right) = \operatorname{Tr}\left(\int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\ \gamma^0\, \widehat{\mathrm{P}^\varepsilon}(p)\right) \tag{5.41}$$

Starting from this definition, we can now study the effect of Lorentz boosts of the velocity of the regularization on the local particle density.

Lemma 5.3.3 (Variation of the Local Particle Density for Lorentz Boosts)

Let $\delta\widehat{\mathrm{P}^\varepsilon}(p)$ and $\delta^2\widehat{\mathrm{P}^\varepsilon}(p)$ be the first and second order variations of the iε-regularized kernel of the fermionic projector corresponding to Lorentz boosts as given in (5.20) and (5.21), respectively. Then the corresponding variation of the local particle density is given by

$$\delta f = 0 \tag{5.42a}$$

$$\delta^2 f = -\frac{2}{(2\pi)^3}\left[\frac{\mu^2}{\varepsilon}\Big(3K_0(\varepsilon\mu) + 4K_2(\varepsilon\mu)\Big) + 2\mu\left(\frac{3}{\varepsilon^2} + \mu^2\right)K_1(\varepsilon\mu)\right] \tag{5.42b}$$

where K_n denote the modified Bessel functions of the second kind. The second variation has a leading-order behaviour which is given by

$$\delta^2 f = -\frac{2}{(2\pi)^3}\left(\frac{14}{\varepsilon^3} - \frac{3\mu^2}{2\varepsilon} + \mathcal{O}(\varepsilon)\right) \tag{5.43}$$

Proof. As the local particle density depends linearly on the regularized kernel of the fermionic projector, the corresponding variations at first and second order are clearly given by

$$\delta f = \operatorname{Tr}\left(\int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\ \gamma^0\, \delta\widehat{\mathrm{P}^\varepsilon}(p)\right) \tag{5.44a}$$

$$\delta^2 f = \operatorname{Tr}\left(\int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\ \gamma^0\, \delta^2\widehat{\mathrm{P}^\varepsilon}(p)\right) \tag{5.44b}$$

By inserting the explicit expression for $\delta\widehat{\mathrm{P}^\varepsilon}(p)$ from (5.20) we find at first order

$$\delta f = \varepsilon \int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\ (\vec{p}\cdot\vec{n}\,)\operatorname{Tr}\left(\gamma^0\, \widehat{\mathrm{P}^\varepsilon}(p)\right) = 4\varepsilon \int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\ (\vec{p}\cdot\vec{n}\,)p^0\delta(p^2-\mu^2)\Theta(-p^0)\mathrm{e}^{\varepsilon p^0} \tag{5.45}$$

where we for the second equality we have used the trace identities $\operatorname{Tr}(\gamma^k\gamma^l) = 4\eta^{kl}$ and $\operatorname{Tr}(\gamma^k) = 0$. To evaluate the remaining integral, we choose the coordinate system in momentum space without loss of generality such that the z-axis coincides with $\vec{n}$. In this way the scalar

[1] For more details, we refer to the discussion of this topic by Finster.[11, Sec. 1.2.1],[6, Sec. 1.2]

[2] Loosely speaking, one basically has to integrate $j^0(0)$ over all momenta and all negative frequencies. For a detailed discussion, we refer to Finster's first book.[6, Sec. 2.6]

product $\vec{p}\cdot\vec{n}$ reduces to $|\vec{p}||\vec{n}|\cos(\theta_p)$ which in turn vanishes upon integration. Thus, the local particle density does not change at first order.

For the second-order calculation we proceed in the same way: By inserting for $\delta^2\widehat{\mathrm{P}^\varepsilon}(p)$ the result obtained in (5.21) and using the trace identities for the Dirac matrices we obtain

$$\delta^2 f = 2\varepsilon \int\limits_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4} \, \Big(p^0 + \varepsilon(\vec{p}\cdot\vec{n}\,)^2\Big) p^0 \delta(p^2-\mu^2)\Theta(-p^0)\mathrm{e}^{\varepsilon p^0} \tag{5.46}$$

Choosing the coordinate system in the same way as before, carrying out the p^0-integral as well as the φ_p-integral and making use of the fact that $\vec{n}$ is a unit vector results in

$$\begin{aligned}\delta^2 f &= -2\pi\varepsilon \int\limits_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4} \int\limits_{-1}^{1} \mathrm{d}\cos(\theta_p)\, \Big(\omega_p + \varepsilon|\vec{p}|^2\cos^2(\theta_p)\Big)\mathrm{e}^{-\varepsilon\omega_p} \\ &= -2\pi\varepsilon \int\limits_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4} \left(2\omega_p + \frac{2}{3}\varepsilon|\vec{p}|^2\right)\mathrm{e}^{-\varepsilon\omega_p}\end{aligned}$$

The remaining integrals can be evaluated using the table of integrals by Gradshteyn and Ryzhik[57, 3.461(1, 2)] such that we finally end up with

$$\begin{aligned}\delta^2 f &= -\frac{4\pi\varepsilon}{(2\pi)^4}\left[-\frac{\partial}{\partial\varepsilon}\left(\frac{2\mu}{\varepsilon^2}K_1(\varepsilon\mu) + \frac{\mu^2}{\varepsilon}K_0(\varepsilon\mu)\right) + \frac{\varepsilon}{3}\left(\frac{12\mu^2}{\varepsilon^3}K_2(\varepsilon\mu) + \frac{3\mu^3}{\varepsilon^2}K_1(\varepsilon\mu)\right)\right] \\ &= -\frac{2}{(2\pi)^3}\left[\frac{3\mu^2}{\varepsilon}K_0(\varepsilon\mu) + \frac{6\mu}{\varepsilon^2}K_1(\varepsilon\mu) + 2\mu^3 K_1(\varepsilon\mu) + \frac{4\mu^2}{\varepsilon}K_2(\varepsilon\mu)\right]\end{aligned} \tag{5.47}$$

Expanding this result around $\varepsilon = 0$ yields the leading-order behaviour which is given by

$$\delta^2 f = -\frac{2}{(2\pi)^3}\left(\frac{14}{\varepsilon^3} - \frac{3\mu^2}{2\varepsilon} + \mathcal{O}(\varepsilon)\right) \tag{5.48}$$

This concludes the proof. □

This lemma demonstrates that Lorentz boosts, although they leave the regularized causal action invariant, nevertheless have an effect on the local particle density of the regularized Dirac sea configuration. More precisely, for non-vanishing mass $\mu > 0$ and regularization length $\varepsilon > 0$ the local particle density (of the Dirac sea) decreases at leading order in the regularization length ε.[3]

[3]This fact, together with some other considerations, forms the starting point for the development of a novel mechanism to explain baryogenesis within the framework of the theory of causal fermion systems.[77]

6

Invertibility of the Second Variation of the Regularized Causal Action

Contents

In this last chapter we focus on the zeroth-order multipole moment of the second variation of the regularized causal action and outline a procedure which allows to construct the inverse of the integral operator $\mathrm{S}^{\varepsilon}_{00}$ from (4.53b) under certain simplifying assumptions.

To better understand the necessity for simplifying assumptions, we briefly recall the achievements from the previous chapters: In Chapter 3 we have derived an expression for $\delta^2\mathcal{S}^{\varepsilon}$ (see (3.31b) in Theorem 3.4.3) which depends on the so-called demarcation function $R^{\varepsilon}_{\max}$. In the homogeneous setting, this function describes the regularization-dependent boundary between spacelike-separated and timelike-separated difference vectors. Through the incomplete Fourier transforms, this demarcation function ultimately enters the integral operators $\mathrm{S}^{\varepsilon}_{lm}$ which describe the multipole moments of the sesquilinear contribution to $\delta^2\mathcal{S}^{\varepsilon}$. Although we were able to simplify the expression for the multipole moments $\delta^2\mathcal{S}^{\varepsilon}_{lm|l'm'}$ by carrying out both the position space angular integrals and the momentum space angular integrals, one problem remained: Due to the fact that the demarcation function $R^{\varepsilon}_{\max}$ is implicitly defined through the condition (2.45), the ξ^0-integral and the r-integral appearing in the integral kernels of $\mathrm{S}^{\varepsilon}_{lm}$ cannot be evaluated, which, in turn, makes it impossible to invert the integral operators $\mathrm{S}^{\varepsilon}_{lm}$ in full generality.

Nevertheless, to make at least a qualitative assessment regarding the invertibility, we consider the zeroth-order multipole moment of $\delta^2\mathcal{S}^{\varepsilon}$ and simplify the above-described setting by specifying the function $R^{\varepsilon}_{\max}$ and taking into account only the most singular contributions of the incomplete Fourier transforms on the lightcone. In this way we are be able to construct a second-order differential operator, serving as the inverse of $\mathrm{S}^{\varepsilon}_{00}$ and to determine its scaling in the regularization length ε.

6.1 Computation of the Integral Operator $\mathrm{S}^{\varepsilon}_{00}$

As mentioned in the above paragraph, the answer to the question whether it is possible to determine the inverses of the integral operators $\mathrm{S}^{\varepsilon}_{lm}$ ultimately depends on the ability to carry out the position space integrals contained in the incomplete Fourier transforms as introduced in Definition 4.2.1. As this proves difficult in full generality, we simplify the setting by using the following observation: The integrands of the incomplete Fourier transforms $\mathcal{F}[(\,\cdot\,)^{\varepsilon}_{lm|l(-m)}]$, namely the corresponding coefficient matrices $\mathcal{C}^{\varepsilon}_{(\cdot)}$, diverge on the lightcone for vanishing regularization while they decay polynomially away from the lightcone both for $|\xi^0| \to \infty$ and $r \to \infty$. As a consequence of this fact, those regions within $\mathcal{R}^{\varepsilon}$ which are closest to the lightcone, account for the dominant contribution to the incomplete Fourier transforms. Thus, by determining the leading-order singularity of the coefficient matrices on the lightcone and by making a reasonable ansatz for the function $R^{\varepsilon}_{\max}$, we are in the position to determine at least the leading-order contribution to the integral operators $\mathrm{S}^{\varepsilon}_{lm}$.

6.1.1 Lightcone Expansion of the Coefficient Matrices

We start by determining the most singular contributions to the coefficient matrices on the lightcone using the lightcone expansion as introduced by Finster[11, Def. 2.2.1]. As we are primarily concerned with a qualitative assessment and since the most singular terms are the same for all four incomplete Fourier transforms appearing in the expression for $\mathrm{S}^{\varepsilon}_{00}$ in (4.53b), we consider, without loss of generality, only the incomplete Fourier transform $\mathcal{F}\big[\mathcal{N}^{\varepsilon}_{00|00}\big]$.

Definition 6.1.1 (Lightcone Expansion of Distributions)

A distribution $A(x, y)$ on $\mathcal{M} \times \mathcal{M}$ is said to be of order $\mathcal{O}((y-x)^{2p})$ for $p \in \mathbb{Z}$, if the product $(y-x)^{-2p} A(x, y)$ is a locally integrable function. An expansion of the form

$$A(x, y) = \sum_{j=g}^{\infty} A^{[j]}(x, y) \quad \text{with} \quad g \in \mathbb{Z} \tag{6.1a}$$

is called *lightcone expansion* if the terms $A^{[j]}(x, y)$ are distributions of order $\mathcal{O}((y-x)^{2j})$ and if A is approximated by the partial sums in the sense that for all $p \geq g$ the distribution

$$A(x, y) - \sum_{j=g}^{p} A^{[j]}(x, y) \tag{6.1b}$$

is of order $\mathcal{O}((y-x)^{2p+2})$.

Based on this definition, we can now determine the leading-order term of the (regularized) lightcone expansion of the coefficient matrix $\mathcal{C}^{\varepsilon}_{\mathcal{N}}$ as given in (4.19b,i). To keep the presentation as clear as possible, we have deferred the detailed computations to Appendix A such that the (regularized) lightcone expansion of the coefficient matrix $\mathcal{C}^{\varepsilon}_{\mathcal{N}}$ follows as a corollary from Lemma A.4.1 and the following Lemma 6.1.2.

Lemma 6.1.2 (Close-to-Lightcone/Away-from-Origin Expansion of $(\Xi^{\varepsilon}_{\mp})^{-2n}$)

In the region which is close to the lightcone (i. e. for $\frac{|\xi^0|-r}{r} \ll 1$) and simultaneously away from the origin (i. e. for $\frac{\varepsilon}{r} \ll 1$), the following expansion holds

$$\frac{1}{(\Xi^{\varepsilon}_{\mp})^{2n}} = \frac{(-1)^n}{(\sqrt{2}\mu r)^{2n}} \left(\frac{|\xi^0|-r}{r}\right)^{-n} \left[1 + (\mp i n)\left[\frac{\epsilon(-\xi^0)}{\frac{|\xi^0|-r}{r}} + \mathcal{O}(1)\right]\frac{\varepsilon}{r} + \mathcal{O}\left(\frac{\varepsilon}{r}\right)^2\right]$$

where $\Xi^\varepsilon_\mp$ denotes the dimensionless variable $\Xi^\varepsilon_\mp = \mu\sqrt{-(\xi^\varepsilon_\mp)^2}$ as defined in (2.36) (with m replaced by μ) and ϵ is the sign function.

Proof. Inserting the definition of $\Xi^\varepsilon_\mp$ from (2.36), factorizing and subsequently expanding in a Taylor series in $\frac{\varepsilon}{r}$ yields

$$\frac{1}{(\Xi^\varepsilon_\mp)^{2n}} = \left[\frac{1}{-\mu^2\big((\xi^0 \mp \mathrm{i}\varepsilon)^2 - r^2\big)}\right]^n$$
$$= \frac{(-1)^n}{(\mu r)^{2n}}\left(\frac{\xi^0 + r}{r}\right)^{-n}\left(\frac{\xi^0 - r}{r}\right)^{-n}\left[1 - (\mp\mathrm{i}n)\left(\frac{1}{\frac{\xi^0+r}{r}} + \frac{1}{\frac{\xi^0-r}{r}}\right)\frac{\varepsilon}{r} + \mathcal{O}\left(\frac{\varepsilon}{r}\right)^2\right]$$

To proceed, we consider the upper lightcone ($\xi^0 > 0$) and the lower lightcone ($\xi^0 < 0$) separately. Rewriting the whole expression in terms of $\frac{\xi^0-r}{r}$ and $\frac{\xi^0+r}{r}$, respectively, and expanding around zero gives

$$\ldots = \frac{(-1)^n}{(\sqrt{2}\mu r)^{2n}}\begin{cases}\left(\frac{\xi^0-r}{r}\right)^{-n}\left[1 + (\mp\mathrm{i}n)\left(-\frac{1}{\frac{\xi^0-r}{r}} + \mathcal{O}(1)\right)\frac{\varepsilon}{r} + \mathcal{O}\left(\frac{\varepsilon}{r}\right)^2\right] & \text{for } \xi^0 > 0\\ (-1)^n\left(\frac{\xi^0+r}{r}\right)^{-n}\left[1 + (\mp\mathrm{i}n)\left(-\frac{1}{\frac{\xi^0+r}{r}} + \mathcal{O}(1)\right)\frac{\varepsilon}{r} + \mathcal{O}\left(\frac{\varepsilon}{r}\right)^2\right] & \text{for } \xi^0 < 0\end{cases}$$

Combining both results, we end up with

$$\ldots = \frac{(-1)^n}{(\sqrt{2}\mu r)^{2n}}\left(\frac{|\xi^0| - r}{r}\right)^{-n}\left[1 + (\mp\mathrm{i}n)\left[\frac{\epsilon(-\xi^0)}{\frac{|\xi^0|-r}{r}} + \mathcal{O}(1)\right]\frac{\varepsilon}{r} + \mathcal{O}\left(\frac{\varepsilon}{r}\right)^2\right]$$

Denoting equality up to higher-order terms in both $\frac{\varepsilon}{r}$ and $\frac{|\xi^0|-r}{r}$ by the symbol $\overset{\circ}{=}$ we thus find

$$\frac{1}{(\Xi^\varepsilon_\mp)^{2n}} \overset{\circ}{=} \frac{(-1)^n}{(\sqrt{2}\mu r)^{2n}}\left(\frac{|\xi^0| - r}{r}\right)^{-n} = \frac{(-1)^n}{(2\mu^2)^n}\frac{(|\xi^0| - r)^{-n}}{r^n}$$

In case there is an additional factor ξ^0 present in the numerator, the leading-order contribution reads

$$\frac{\xi^0}{(\Xi^\varepsilon_\mp)^{2n}} \overset{\circ}{=} \frac{(-1)^n\epsilon(\xi^0)}{(2\mu^2)^n}\frac{(|\xi^0| - r)^{-n}}{r^{n-1}}$$

where we have used the expansion

$$\xi^0 = r\cdot\frac{\xi^0 + r - r}{r} = r \times \begin{cases}1 + \frac{\xi^0-r}{r} & \text{for } \xi^0 > 0\\ -1 + \frac{\xi^0+r}{r} & \text{for } \xi^0 < 0\end{cases}$$

This concludes the proof. □

Combining this expansion with the result from Lemma A.4.1 we arrive at the following close-to-the-lightcone/away-from-the-origin expansion of the coefficient matrix $\mathcal{C}^\varepsilon_\mathcal{N}$.[1]

Corollary 6.1.3 (CTL/AFO Expansion of the Coefficient Matrix $\mathcal{C}^\varepsilon_\mathcal{N}$)

Let $\mathcal{C}^\varepsilon_\mathcal{N}$ be the coefficient matrix as given in (4.19b,i) and customized to the iε-regularization which corresponds to the incomplete Fourier transform $\mathcal{F}[\mathcal{N}^\varepsilon_{lm|l(-m)}]$. The leading-order term

[1] As an abbreviation for the lengthy term "close-to-the-lightcone/away-from-the-origin expansion" we will from now on use the shortcut CTL/AFO expansion.

in the CTL/AFO expansion of the matrix is given by

$$\mathcal{C}^{\varepsilon}_{\mathcal{N}} = \frac{1}{(2\pi)^6} \frac{(|\xi^0| - r)^{-4}}{4r^3} \begin{pmatrix} -r & \epsilon(\xi^0)\mathbb{1}_{1\times 3} & 0 \\ \epsilon(\xi^0)\mathbb{1}_{3\times 1} & -\frac{1}{r}\mathbb{1}_{3\times 3} & 0_{3\times 1} \\ 0 & 0_{1\times 3} & 0 \end{pmatrix} \tag{6.2}$$

Proof. To arrive at the claimed expression, we first have to customize the vector and scalar components v^{ε}_0, v^{ε}_i, s^{ε} of the regularized kernel of the fermionic projector to the case of the iε-regularization which, by comparing the general vector-scalar structure in (3.9) with the one for the iε-regularized kernel of the fermionic projector in (2.37), amounts to the following replacements

$$v^{\varepsilon}_i(x,y) \to (\xi^{\varepsilon}_-)_i g^{\varepsilon}_-(\xi) \overset{\text{(A.5a)}}{=} (\xi^{\varepsilon}_-)_i \tilde{g}_-(\Xi^{\varepsilon}_-) \qquad \text{and} \qquad s^{\varepsilon}(x,y) \to h^{\varepsilon}_-(\xi) \overset{\text{(A.5b)}}{=} \tilde{h}(\Xi^{\varepsilon}_-) \tag{6.3}$$

Together with the abbreviating notation introduced in Appendix Section A.3 and the definition of the function B^{ε} from (3.15), the coefficient matrix $\mathcal{C}^{\varepsilon}_{\mathcal{N}}$ becomes

$$\mathcal{C}^{\varepsilon}_{\mathcal{N}} \overset{\text{(A.20)}}{=} \begin{pmatrix} -r^2|g|^2 + |h|^2 & -((\xi^{\varepsilon}_+)^0 - 2(\xi^{\varepsilon}_-)^0)|g|^2\mathbb{1}_{1\times 3} & (\xi^{\varepsilon}_+)^0\bar{g}h + 2(\xi^{\varepsilon}_-)^0 g\bar{h} \\ -((\xi^{\varepsilon}_-)^0 - 2(\xi^{\varepsilon}_+)^0)|g|^2\mathbb{1}_{3\times 1} & -|g|^2\mathbb{1}_{3\times 3} & -(\bar{g}h + 2g\bar{h})\mathbb{1}_{3\times 1} \\ (\xi^{\varepsilon}_-)^0 g\bar{h} + 2(\xi^{\varepsilon}_+)^0\bar{g}h & -(g\bar{h} + 2\bar{g}h)\mathbb{1}_{1\times 3} & |\xi^{\varepsilon}|^2|g|^2 \end{pmatrix} \tag{6.4}$$

Next, by using the leading-order contributions of the component functions $\tilde{g}_{\mp}$ and $\tilde{h}$ as derived in (A.20) in Lemma A.4.1, we obtain

$$\mathcal{C}^{\varepsilon}_{\mathcal{N}} = \frac{4\mu^8}{(2\pi)^6}\frac{1}{|\Xi^{\varepsilon}|^4} \begin{pmatrix} -\frac{r^2}{|\Xi^{\varepsilon}|^4} & -\frac{(\xi^{\varepsilon}_+)^0 - 2(\xi^{\varepsilon}_-)^0}{|\Xi^{\varepsilon}|^4}\mathbb{1}_{1\times 3} & \frac{\mathrm{i}}{2\mu}\Big(\frac{(\xi^{\varepsilon}_+)^0}{(\Xi^{\varepsilon}_+)^2} - \frac{2(\xi^{\varepsilon}_-)^0}{(\Xi^{\varepsilon}_-)^2}\Big) \\ -\frac{(\xi^{\varepsilon}_-)^0 - 2(\xi^{\varepsilon}_+)^0}{|\Xi^{\varepsilon}|^4}\mathbb{1}_{3\times 1} & -\frac{1}{|\Xi^{\varepsilon}|^4}\mathbb{1}_{3\times 3} & -\frac{\mathrm{i}}{2\mu}\Big(\frac{1}{(\Xi^{\varepsilon}_+)^2} - \frac{2}{(\Xi^{\varepsilon}_-)^2}\Big)\mathbb{1}_{3\times 1} \\ \frac{\mathrm{i}}{2\mu}\Big(-\frac{(\xi^{\varepsilon}_-)^0}{(\Xi^{\varepsilon}_-)^2} + \frac{2(\xi^{\varepsilon}_+)^0}{(\Xi^{\varepsilon}_+)^2}\Big) & -\frac{\mathrm{i}}{2\mu}\Big(-\frac{1}{(\Xi^{\varepsilon}_-)^2} + \frac{2}{(\Xi^{\varepsilon}_+)^2}\Big)\mathbb{1}_{1\times 3} & \frac{|\xi^{\varepsilon}|^2}{|\Xi^{\varepsilon}|^4} \end{pmatrix} \tag{6.5}$$

where we kept the leading-order contributions *in each entry.* Making use of the expansion in Lemma 6.1.2 we finally arrive at

$$\mathcal{C}^{\varepsilon}_{\mathcal{N}} \overset{\circ}{=} \frac{1}{(2\pi)^6}\frac{(|\xi^0| - r)^{-3}}{4r^3} \begin{pmatrix} -\frac{r}{(|\xi^0|-r)} & \frac{\epsilon(\xi^0)}{(|\xi^0|-r)}\mathbb{1}_{1\times 3} & \mathrm{i}\mu r\cdot\epsilon(\xi^0) \\ \frac{\epsilon(\xi^0)}{(|\xi^0|-r)}\mathbb{1}_{3\times 1} & -\frac{1}{r}\frac{1}{(|\xi^0|-r)}\mathbb{1}_{3\times 3} & -\mathrm{i}\mu\mathbb{1}_{3\times 1} \\ -\mathrm{i}\mu r\cdot\epsilon(\xi^0) & \mathrm{i}\mu\mathbb{1}_{1\times 3} & 1 \end{pmatrix} \tag{6.6}$$

As can be seen from this expression, the leading-order contribution of the matrix *as a whole* is given by the matrix where all entries except for those in the upper left (4×4)-block matrix are zero.

This concludes the proof. □

6.1.2 Weak Evaluation of the Coefficient Matrix on the Lightcone

Having determined the leading-order contribution of the coefficient matrix $\mathcal{C}^{\varepsilon}_{\mathcal{N}}$ in the CTL/AFO expansion, the next step consists in modelling the behaviour of the resulting incomplete Fourier transform $\mathcal{F}[\mathcal{N}^{\varepsilon}_{lm|l(-m)}]$ near the lightcone. To this end we make use of the so-called *weak evaluation on the lightcone* which is an integral part of the *formalism of the continuum limit* as introduced by Finster.[6, Ch. 4]. In an nutshell, this formalism arises from the necessity to analyze the regularization-dependence of the Euler-Lagrange equations in order to establish the connection with contemporary physics.[2] For our purposes, however, we do not need the full machinery of the formalism of the continuum limit, except for the weak evaluation on the lightcone which allows to quantify the singular behaviour of regularized expressions in the limit $\varepsilon \searrow 0$. Technically, the weak evaluation on the lightcone is implemented by integrating the respective regularization-dependent expression (which in the limit $\varepsilon \searrow 0$ diverges on the lightcone) against a smooth test function with respect to ξ^0 for fixed r. Applying this concept in a slightly modified form to the leading-order term in the CTL/AFO expansion of $(\Xi^\varepsilon_\mp)^{-2n}$ as derived in Lemma 6.1.2 leads to the following result.

Lemma 6.1.4 (Weak Evaluation of $(\Xi^\varepsilon_\mp)^{-2n}$ on the Lightcone)

Let the regularization be chosen such that the demarcation function $R_{\max}$ as introduced in Definition 2.3.8 takes the form

$$R^\varepsilon_{\max}(\xi^0) = \xi^0 - c\varepsilon^d \qquad \text{with} \qquad c > 0,\, d \in (0,1) \tag{6.7}$$

away from the origin.[a] Then, weakly evaluating the functions $(|\xi^0| - r)^{-n} r^{-m}$ and $\epsilon(\xi^0)(|\xi^0| - r)^{-n} r^{-m}$ on the lightcone amounts to simultaneously replacing

$$\int_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0, r) \to \int_{\mathbb{R}} \mathrm{d}\xi^0 \int_0^\infty \mathrm{d}r \tag{6.8a}$$

and

$$\frac{(|\xi^0| - r)^{-n}}{r^m} \begin{Bmatrix} 1 \\ \epsilon(\xi^0) \end{Bmatrix} \to \frac{(c\varepsilon^d)^{1-n}}{n-1} \frac{\delta(\xi^2)\epsilon(\xi^0)^{m-1}}{(\xi^0)^{m-1}} \begin{Bmatrix} 1 \\ \epsilon(\xi^0) \end{Bmatrix} \tag{6.8b}$$

where ϵ denotes the sign function.

Proof. According to the preceding paragraph, the weak evaluation on the lightcone aims at analyzing the singular behavior of a regularization-dependent expression on the lightcone by determining its scaling in the regularization length ε. In our case, where we are interested in evaluating incomplete Fourier transforms, namely integrals of the form

$$\int_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0, r)\ \frac{(|\xi^0| - r)^{-n}}{r^m} \begin{Bmatrix} 1 \\ \epsilon(\xi^0) \end{Bmatrix} f(kr)\mathrm{e}^{-\mathrm{i}\omega\xi^0} \tag{6.9}$$

the setting is slightly different: Unlike usual, here the regularization is encoded in the domain of integration instead of the integrand. Nevertheless, the basic idea remains the same: In order to determine the scaling in ε, we fix $r \gg \varepsilon$ and integrate in ξ^0-direction. For $n \geq 2$ we obtain in this way

$$\begin{aligned}
&\int_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0, r)\ \frac{(|\xi^0| - r)^{-n}}{r^m} \begin{Bmatrix} 1 \\ \epsilon(\xi^0) \end{Bmatrix} = \\
&= \int_0^\infty \mathrm{d}r\ \frac{1}{r^m} \left((-1)^n \int_{-\infty}^{-T_{\min}(r)} \mathrm{d}\xi^0\ (\xi^0 + r)^{-n} \begin{Bmatrix} 1 \\ \epsilon(\xi^0) \end{Bmatrix} + \int_{T_{\min}(r)}^\infty \mathrm{d}\xi^0\ (\xi^0 - r)^{-n} \begin{Bmatrix} 1 \\ \epsilon(\xi^0) \end{Bmatrix} \right) \\
&= \int_0^\infty \mathrm{d}r\ \frac{1}{r^m} \left((-1)^n \begin{Bmatrix} 1 \\ -1 \end{Bmatrix} \left[\frac{(\xi^0 + r)^{-n+1}}{-n+1} \right]_{-\infty}^{-T_{\min}(r)} + \left[\frac{(\xi^0 - r)^{-n+1}}{-n+1} \right]_{T_{\min}(r)}^\infty \right)
\end{aligned}$$

[2]For the development of a deeper understanding of the formalism of the continuum limit we warmly recommend the insightful, but rarely mentioned discussions by Finster[6, Sec. 3.6], [6, Sec. 4.1, 4.2], along with the computations in [6, Sec. 4.3 - 4.5]. In order to get a first, rough overview, however, we refer to the explanations given in [11, Sec. 2.4.1] and [11, Sec. 2.4.4] together with the introductory paragraph of [11, Sec. 2.4].

$$= \int_0^\infty \mathrm{d}r \; \frac{1}{r^m}\left(\begin{Bmatrix}1\\-1\end{Bmatrix}(-1)^n \frac{\big(-T_{\min}(r)+r\big)^{-n+1}}{-n+1} - \frac{\big(T_{\min}(r)-r\big)^{-n+1}}{-n+1}\right)$$
$$= \int_0^\infty \mathrm{d}r \; \frac{1}{r^m}\left(\begin{Bmatrix}1\\-1\end{Bmatrix}+1\right)\frac{\big(T_{\min}(r)-r\big)^{1-n}}{n-1}$$

where we used that the boundary terms for $\xi^0 \to \pm\infty$ vanish identically. Choosing the regularization such that the function $R^{\varepsilon}_{\max}(\xi^0)$ is given by $R^{\varepsilon}_{\max}(\xi^0) = \xi^0 - c\varepsilon^d$ away from the lightcone which translates into $T_{\min}(r) = r + c\varepsilon^d$ for $r > R^{\varepsilon}_{\max}(0)$, we obtain[b]

$$\int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0, r) \;\; \frac{(|\xi^0|-r)^{-n}}{r^m}\begin{Bmatrix}1\\ \epsilon(\xi^0)\end{Bmatrix} = \int_0^\infty \mathrm{d}r \; \frac{(c\varepsilon^d)^{1-n}}{n-1}\frac{1}{r^m}\begin{Bmatrix}1\\0\end{Bmatrix}$$

Thus, away from the origin but on the lightcone, the expressions $(|\xi^0|-r)^{-n}r^{-m}$ and $\epsilon(\xi^0)(|\xi^0|-r)^{-n}r^{-m}$ can be modelled by simultaneously replacing

$$\int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0, r) \;\to\; \int_{\mathbb{R}} \mathrm{d}\xi^0 \int_0^\infty \mathrm{d}r$$

and

$$\frac{(|\xi^0|-r)^{-n}}{r^m}\begin{Bmatrix}1\\ \epsilon(\xi^0)\end{Bmatrix} \to \frac{(c\varepsilon^d)^{1-n}}{n-1}\frac{\delta(\xi^2)\epsilon(\xi^0)^{m-1}}{(\xi^0)^{m-1}}\begin{Bmatrix}1\\ \epsilon(\xi^0)\end{Bmatrix}$$

This concludes the proof. □

[a] Note that the parameter c must have length dimension $\dim(c) = 1-d$ in order to ensure that $R^{\varepsilon}_{\max}$ has length dimension $\dim(R^{\varepsilon}_{\max}) = 1$.

[b] Note that in the lower case the expression vanishes due to the fact that the contributions for $\xi^0 > 0$ and $\xi^0 < 0$ are non-vanishing but cancel each other.

6.1.3 Computing the Weakly Evaluated Incomplete Fourier Transforms

So far we have worked out the lightcone expansion of the coefficient matrix $\mathcal{C}^{\varepsilon}_{\mathcal{N}}$ and demonstrated how its leading-order singularity on the lightcone can be modelled. With these results at hand we are now able to compute the simplified position space integrals in Lemma 4.2.12 which leads us to a manageable expression for the incomplete Fourier transform $\mathcal{F}[\mathcal{N}^{\varepsilon}_{00|00}]$.

Proposition 6.1.5 (Computation of Weakly Evaluated Fourier Integrals)

For any $m \in \mathbb{N}$ the integral functions $I^f_{\upuparrows\downarrow|m} : \mathbb{R}^2 \to \mathbb{R}$ defined as

$$I^f_{\upuparrows\downarrow|m}(\omega, k) := \int_{\mathbb{R}} \mathrm{d}\xi^0 \int_0^\infty \mathrm{d}r \;\; \frac{\delta(\xi^2)\epsilon(\xi^0)^{m-1}}{(\xi^0)^{m-1}} f(kr)\mathrm{e}^{-\mathrm{i}\omega\xi^0}\begin{Bmatrix}1\\ \epsilon(\xi^0)\end{Bmatrix} \tag{6.11a}$$

where the arrows refer to the upper and lower case, respectively, evaluate to Fourier cosine transforms and Fourier sine transforms of the function $\frac{f(kr)}{r^m}$

$$I^f_{\uparrow|m}(\omega, k) = \mathcal{F}_{\cos}\left(\frac{f(kr)}{r^m}\right)(\omega) \qquad \text{and} \qquad I^f_{\downarrow|m}(\omega, k) = -\mathrm{i}\mathcal{F}_{\sin}\left(\frac{f(kr)}{r^m}\right)(\omega) \tag{6.11b}$$

Proof. To prove the claimed relations, we start by rewriting the Dirac delta distribution using the rule for composition with another function and thus obtain

$$I^f_{\uparrow\!\downarrow|m}(\omega,k) = \int_{\mathbb{R}} \mathrm{d}\xi^0 \int_0^\infty \mathrm{d}r\; \frac{\mathrm{e}^{-\mathrm{i}\omega\xi^0}}{(\xi^0)^{m-1}} \frac{f(kr)}{2r} \Big[\delta(\xi^0+r)+\delta(\xi^0-r)\Big]\epsilon(\xi^0)^{m-1} \begin{Bmatrix} 1 \\ \epsilon(\xi^0) \end{Bmatrix}$$

Carrying out the ξ^0-integral in the two different cases results in

$$\begin{aligned} \ldots &= \int_0^\infty \mathrm{d}r\; \frac{f(kr)}{2r} \times \begin{Bmatrix} (-1)^{m-1}\frac{\mathrm{e}^{-\mathrm{i}\omega(-r)}}{(-r)^{m-1}} + \frac{\mathrm{e}^{-\mathrm{i}\omega r}}{r^{m-1}} \\ -(-1)^{m-1}\frac{\mathrm{e}^{-\mathrm{i}\omega(-r)}}{(-r)^{m-1}} + \frac{\mathrm{e}^{-\mathrm{i}\omega r}}{r^{m-1}} \end{Bmatrix} \\ &= \int_0^\infty \mathrm{d}r\; \frac{f(kr)}{r^m} \times \begin{cases} \cos(\omega r) & \text{for } \uparrow \\ -\mathrm{i}\sin(\omega r) & \text{for } \downarrow \end{cases} \end{aligned}$$

This result demonstrates that the integral functions $I^f_{\uparrow\!\downarrow|m}$ can be interpreted as the Fourier cosine transform (for $\uparrow$) and the Fourier sine transform (for $\downarrow$) of the function $f(kr)r^{-m}$ with respect to the variable ω

$$I^f_{\uparrow|m}(\omega,k) = \mathcal{F}_{\cos}\left(\frac{f(kr)}{r^m}\right)(\omega) \qquad \text{and} \qquad I^f_{\downarrow|m}(\omega,k) = -\mathrm{i}\mathcal{F}_{\sin}\left(\frac{f(kr)}{r^m}\right)(\omega) \tag{6.12}$$

This concludes the proof. □

According to Lemma 4.2.12, the position space integrals also involve the multipole matrices $\mathfrak{M}_{ll}$, $\mathfrak{N}_{ll}$ as well as their asterisked counterparts $\overset{*}{\mathfrak{M}}_{ll}$ and $\overset{*}{\mathfrak{N}}_{ll}$ which all carry an r-dependence through sines and cosines (see Appendix E.1). This means that the integral functions $I^f_{\uparrow\!\downarrow|m}$ have to be evaluated for $f \in \{\cos,\sin\}$ and, in the case relevant for us, for $m \in \{2,3,4\}$.

Lemma 6.1.6 (Evaluation of Integral Functions $I^f_{\uparrow\!\downarrow|m}$ for $f \in \{\cos,\sin\}$)

For $f \in \{\cos,\sin\}$ and $m \in \{2,3,4\}$ the integral functions $I^f_{\uparrow|m}$ as introduced in Proposition 6.1.5 evaluate to

$$\frac{2}{\pi} I^{\cos}_{\uparrow|2}(\omega,k) = -\frac{|\omega-k|+|\omega+k|}{2} = \begin{cases} -|\omega| & \text{for } |\omega|>|k| \\ -|k| & \text{for } |k|\geq|\omega| \end{cases} \tag{6.13a}$$

$$\frac{2}{\pi} I^{\cos}_{\uparrow|4}(\omega,k) = \frac{|\omega-k|^3+|\omega+k|^3}{12} = \begin{cases} \frac{|\omega|}{6}(\omega^2+3k^2) & \text{for } |\omega|>|k| \\ \frac{|k|}{6}(3\omega^2+k^2) & \text{for } |\omega|\leq|k| \end{cases} \tag{6.13b}$$

$$\frac{2}{\pi} I^{\sin}_{\uparrow|3}(\omega,k) = \frac{|\omega-k|(\omega-k)-|\omega+k|(\omega+k)}{4} = \begin{cases} \epsilon(-k)|\omega||k| & \text{for } |\omega|>|k| \\ \frac{\epsilon(-k)}{2}(\omega^2+k^2) & \text{for } |\omega|\leq|k| \end{cases} \tag{6.13c}$$

while for $I^f_{\downarrow|m}$ we analogously obtain

$$\frac{2}{\pi} I^{\cos}_{\downarrow|3}(\omega,k) = \mathrm{i}\frac{|\omega-k|(\omega-k)+|\omega+k|(\omega+k)}{4} = \begin{cases} \mathrm{i}\frac{\epsilon(\omega)}{2}(\omega^2+k^2) & \text{for } |\omega|>|k| \\ \mathrm{i}\epsilon(\omega)|\omega||k| & \text{for } |\omega|\leq|k| \end{cases} \tag{6.13d}$$

$$\frac{2}{\pi} I^{\sin}_{\downarrow|2}(\omega,k) = \mathrm{i}\frac{|\omega-k|-|\omega+k|}{2} = \begin{cases} \mathrm{i}\epsilon(-\omega)\epsilon(k)|k| & \text{for } |\omega|>|k| \\ \mathrm{i}\epsilon(-\omega)\epsilon(k)|\omega| & \text{for } |\omega|\leq|k| \end{cases} \tag{6.13e}$$

Proof. To prove the claimed relations, we first of all remark that Fourier sine and cosine transforms as defined in (6.11b) are related via

$$-\mathrm{i}I^{\sin}_{\uparrow|m}(k,\omega) = I^{\cos}_{\downarrow|m}(\omega,k)$$

which directly implies that (6.13d) can be obtained from (6.13c) by interchanging arguments. In addition to this, we furthermore have the relations

$$\frac{\partial I^{\cos}_{\uparrow\!\downarrow|m+1}(\omega,k)}{\partial k} = -I^{\sin}_{\uparrow\!\downarrow|m}(\omega,k) \qquad \text{and} \qquad \frac{\partial I^{\sin}_{\uparrow\!\downarrow|m+1}(\omega,k)}{\partial k} = I^{\cos}_{\uparrow\!\downarrow|m}(\omega,k)$$

as well as

$$\frac{\partial I^{\bullet}_{\uparrow|m+1}(\omega,k)}{\partial \omega} = -I^{\bullet}_{\downarrow|m}(\omega,k) \qquad \text{and} \qquad \frac{\partial I^{\bullet}_{\downarrow|m+1}(\omega,k)}{\partial \omega} = I^{\bullet}_{\uparrow|m}(\omega,k)$$

which allows to obtain both (6.13a) and (6.13e) from (6.13c) (or, equivalently, from (6.13d)). Finally, by the same reasoning, we observe that (6.13c) (and, likewise, (6.13d)) can be computed from (6.13b) which is sufficient to produce all claimed expressions via the above relations. Evaluating $I^{f}_{\uparrow\!\downarrow|m}(\omega,k)$ for $f \in \{\cos,\sin\}$ by using the commands `FourierCosTransform` and `FourierSinTransform` implemented in `Mathematica 12` gives the result.[a]

For the sake of completeness we remark that the integral functions $I^{\bullet}_{\uparrow\!\downarrow|m}(\omega,k)$ must be understood in the distributional sense. The necessity for a distributional treatment can already be recognized by trying to compute $I^{\cos}_{\uparrow\!\downarrow|2}(\omega,k)$ naively

$$\begin{aligned} I^{\cos}_{\uparrow\!\downarrow|2}(\omega,k) &= \int_0^\infty \mathrm{d}r\, \frac{\cos(\omega r)\cos(kr)}{r^2} = \int_0^\infty \mathrm{d}r\, \frac{\cos[(\omega-k)r]+\cos[(\omega+k)r]}{2r^2} \\ &= -\int_0^\infty \mathrm{d}r\, \frac{\sin^2\left[\frac{\omega-k}{2}r\right]+\sin^2\left[\frac{\omega+k}{2}r\right]}{r^2} + \int_0^\infty \mathrm{d}r\, \frac{1}{r^2} \end{aligned}$$

where we exploited the double-angle formula $\cos(x) = 1 - 2\sin^2(x/2)$ in the last step. Making use of the identity $\int_0^\infty \mathrm{d}x\, \sin^2(ax)/x^2 = \frac{\pi}{2}a$ which holds for $a > 0$[57, 3.821(9)], we obtain

$$\frac{2}{\pi} I^{\cos}_{\uparrow\!\downarrow|2}(\omega,k) = -\frac{|\omega-k|+|\omega+k|}{2} + \frac{2}{\pi}\int_0^\infty \mathrm{d}r\, \frac{1}{r^2}$$

which differs from the desired, finite result by an infinite constant. As one could have already anticipated form the very definition of $I^{\cos}_{\uparrow\!\downarrow|2}(\omega,k)$, this divergence traces back to the sharp singularity of the integrand at $r = 0$. The correct way to avoid the appearance of this constant in the first place is to regularize $I^{\cos}_{\uparrow\!\downarrow|2}(\omega,k)$ using Hadamard's method of dropping divergent terms and keeping only the finite parts.[79, Book III, Ch. 2],[b] □

[a] Note that the commands `FourierSinTransform` and `FourierCosTransform` include an additional factor $(2/\pi)^{1/2}$ compared with our definition. Explicitly, the command `FourierCosTransform` and $I^{f}_{\uparrow|m}(\omega,k)$ are related via

$$I^{f}_{\uparrow|m}(\omega,k) = (2/\pi)^{1/2}\, \texttt{FourierCosTransform}\big[f(kr)/r^m, r, \omega\big] \tag{6.14}$$

and similarly for the Fourier sine transform.

[b] For a systematic and detailed treatment of Hadamard's finite part and its relation to the Cauchy principal value, we refer to the book by Kanwal.[80, Sec. 4.2] Note that similar integrals, namely $I^{1}_{\uparrow\!\downarrow|1}(\omega,k)$, $I^{1}_{\uparrow\!\downarrow|2}(\omega,k)$ and derivatives thereof, have already been computed by Finster[81], though with another method where the integral functions in Proposition 6.1.5 are treated differently compared with our approach.

With these results at hand, we are now ready to compute the angular-integrated incomplete Fourier transform $\mathcal{F}\big[\mathcal{N}^{\varepsilon}_{00|00}\big](|\vec{p}|,|\vec{q}|)$ under the simplifying assumptions discussed above.

Lemma 6.1.7 (Incomplete Fourier Transform for Weakly Evaluated Integrand)

The incomplete Fourier transform $\mathcal{F}\big[\mathcal{N}^{\varepsilon}_{00|00}\big](|\vec{p}|,|\vec{q}|)$ from (4.44b) with its integrand replaced by the weakly evaluated, leading-order contribution on the lightcone is given by

$$\mathcal{F}\big[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}\big](|\vec{p}|,|\vec{q}|) = \frac{1/3}{(2\pi)^3}\,\frac{(c\varepsilon^d)^{-3}}{\omega_p\omega_q}\left(\begin{array}{cc|c} -\min\left\{\frac{1}{|\vec{p}|},\frac{1}{|\vec{q}|}\right\} & \min\left\{0,\frac{|\vec{p}|}{|\vec{q}|^2}\frac{\omega_p-\omega_q}{|\vec{p}|}\right\} & \\ \min\left\{0,\frac{|\vec{q}|}{|\vec{p}|^2}\frac{\omega_q-\omega_p}{|\vec{q}|}\right\} & -\frac{1}{3}\frac{\min\left\{\frac{|\vec{p}|^2}{|\vec{q}|},\frac{|\vec{q}|^2}{|\vec{p}|}\right\}}{|\vec{p}||\vec{q}|} & \mathbf{0}_{2\times 3} \\ \hline \multicolumn{2}{c|}{\mathbf{0}_{3\times 2}} & \mathbf{0}_{3\times 3} \end{array}\right) \tag{6.15}$$

where we have $d\in(0,1)$ as introduced in Lemma 6.1.4,

Proof. In order to derive the claimed expression, we start by recalling the explicit form of the angular-integrated incomplete Fourier transform $\mathcal{F}\big[\mathcal{N}^{\varepsilon}_{00|00}\big](|\vec{p}|,|\vec{q}|)$ which according to (4.44b) is given by

$$\mathcal{F}\big[\mathcal{N}^{\varepsilon}_{00|00}\big](|\vec{p}|,|\vec{q}|) \overset{(4.44b)}{=} \int_{\mathfrak{X}^{\varepsilon}} \mathrm{d}(\xi^0,r)\; r^2 E^{\varepsilon}_{\mathcal{N}}\big(\mathfrak{C}^{\varepsilon}_{\mathcal{N}}\odot\mathfrak{N}_{00} - B^{\varepsilon}\overset{*}{\mathfrak{N}}_{00}\big)$$

To compute the integral, we now make use of the groundwork carried out in the previous sections: First, we take into account only the leading-order term of $\mathfrak{C}^{\varepsilon}_{\mathcal{N}}$ in the lightcone expansion as derived in Corollary 6.1.3. Concerning the prefactor B^{ε} of the asterisked term we remark that it is of next-to-leading-order compared with $\mathfrak{C}^{\varepsilon}_{\mathcal{N}}$ and thus irrelevant for our considerations. Next, by inserting the definition of $E^{\varepsilon}_{\mathcal{N}}$ from (4.19b,ii) along with the explicit form of $\mathfrak{N}_{00}$ as given in (E.2a) and the leading-order contribution of $\mathfrak{C}^{\varepsilon}_{\mathcal{N}}$ from (6.2) we find

$$\begin{aligned}\mathcal{F}\big[\mathcal{N}^{\varepsilon}_{00|00}\big](|\vec{p}|,|\vec{q}|) &\overset{(4.19b,ii)}{\underset{(E.2a)}{=}} \frac{1}{(2\pi)^4}\,\frac{2}{\omega_p\omega_q|\vec{p}||\vec{q}|}\int_{\mathfrak{X}^{\varepsilon}}\mathrm{d}(\xi^0,r)\;\frac{(|\xi^0|-r)^{-4}}{r^3}\mathrm{e}^{-\mathrm{i}(\omega_p-\omega_q)\xi^0}\times\\ &\times\Bigg[\left(\begin{array}{cc|c} r & -\frac{\mathrm{i}\epsilon(\xi^0)}{|\vec{q}|} & \\ \frac{\mathrm{i}\epsilon(\xi^0)}{|\vec{p}|} & \frac{1}{r}\frac{1-|\vec{p}||\vec{q}|r^2}{|\vec{p}||\vec{q}|} & \mathbf{0}_{2\times 3} \\ \hline \multicolumn{2}{c|}{\mathbf{0}_{3\times 2}} & \mathbf{0}_{3\times 3}\end{array}\right)\cos\big[(|\vec{p}|+|\vec{q}|)r\big] + \left(\begin{array}{cc|c} -r & \frac{\mathrm{i}\epsilon(\xi^0)}{|\vec{q}|} & \\ -\frac{\mathrm{i}\epsilon(\xi^0)}{|\vec{p}|} & -\frac{1}{r}\frac{1+|\vec{p}||\vec{q}|r^2}{|\vec{p}||\vec{q}|} & \mathbf{0}_{2\times 3} \\ \hline \multicolumn{2}{c|}{\mathbf{0}_{3\times 2}} & \mathbf{0}_{3\times 3}\end{array}\right)\cos\big[(|\vec{p}|-|\vec{q}|)r\big]\\ &\quad+\left(\begin{array}{cc|c} 0 & -\mathrm{i}r\epsilon(\xi^0) & \\ \mathrm{i}r\epsilon(\xi^0) & \frac{|\vec{p}|+|\vec{q}|}{|\vec{p}||\vec{q}|} & \mathbf{0}_{2\times 3} \\ \hline \multicolumn{2}{c|}{\mathbf{0}_{3\times 2}} & \mathbf{0}_{3\times 3}\end{array}\right)\sin\big[(|\vec{p}|+|\vec{q}|)r\big] + \left(\begin{array}{cc|c} 0 & -\mathrm{i}r\epsilon(\xi^0) & \\ -\mathrm{i}r\epsilon(\xi^0) & -\frac{|\vec{p}|-|\vec{q}|}{|\vec{p}||\vec{q}|} & \mathbf{0}_{2\times 3} \\ \hline \multicolumn{2}{c|}{\mathbf{0}_{3\times 2}} & \mathbf{0}_{3\times 3}\end{array}\right)\sin\big[(|\vec{p}|-|\vec{q}|)r\big]\Bigg]\end{aligned}$$

Having arrived at this point, the next step is to weakly evaluate the integrand on the lightcone as explained in Lemma 6.1.4. Subsequently, by evaluating the resulting integrals using Proposition 6.1.5 and Lemma 6.1.6, we obtain

$$\mathcal{F}\big[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}\big](|\vec{p}|,|\vec{q}|) = \frac{2/3}{(2\pi)^4}\,\frac{(c\varepsilon^d)^{-3}}{\omega_p\omega_q|\vec{p}||\vec{q}|}\begin{pmatrix} I^{\cos}_{\uparrow|2}(\omega,k_+) - I^{\cos}_{\uparrow|2}(\omega,k_-) & \begin{array}{r}-\mathrm{i}\Big[\frac{1}{|\vec{q}|}\big(I^{\cos}_{\downarrow|3}(\omega,k_+)-I^{\cos}_{\downarrow|3}(\omega,k_-)\big)\\ +\big(I^{\sin}_{\downarrow|2}(\omega,k_+)+I^{\sin}_{\downarrow|2}(\omega,k_-)\big)\Big]\end{array} \\ \begin{array}{r}\mathrm{i}\Big[\frac{1}{|\vec{p}|}\big(I^{\cos}_{\downarrow|3}(\omega,k_+)-I^{\cos}_{\downarrow|3}(\omega,k_-)\big)\\ +\big(I^{\sin}_{\downarrow|2}(\omega,k_+)-I^{\sin}_{\downarrow|2}(\omega,k_-)\big)\Big]\end{array} & \begin{array}{r}\frac{1}{|\vec{p}||\vec{q}|}\big(I^{\cos}_{\uparrow|4}(\omega,k_+)-I^{\cos}_{\uparrow|4}(\omega,k_-)\big)-\big(I^{\cos}_{\uparrow|2}(\omega,k_+)+I^{\cos}_{\uparrow|2}(\omega,k_-)\big)\\ +\frac{1}{|\vec{q}|}\big(I^{\sin}_{\uparrow|3}(\omega,k_+)-I^{\sin}_{\uparrow|3}(\omega,k_-)\big)+\frac{1}{|\vec{p}|}\big(I^{\sin}_{\uparrow|3}(\omega,k_+)+I^{\sin}_{\uparrow|3}(\omega,k_-)\big)\end{array}\end{pmatrix}$$

where we suppressed the zero rows and columns and defined $\omega := \omega_p - \omega_q$ and $k_\pm := |\vec{p}|\pm|\vec{q}|$.

It remains to further simplify the matrix entries by evaluating the expression in the two cases $|\vec{p}|>|\vec{q}|$ and $|\vec{p}|<|\vec{q}|$, each for $|\vec{p}|,|\vec{q}|\geq 0$. To this end we first note that the functions $f_\pm(|\vec{p}|) := \omega_p \pm |\vec{p}| = \sqrt{|\vec{p}|^2+\mu^2}\pm|\vec{p}|$ both start from $f_\pm(0)=\mu>0$ and are strictly increasing (for f_+) and strictly decreasing (for f_-) on $\mathbb{R}^+_0$. As a consequence, both the relations

$$\omega_p - |\vec{p}| \leq \omega_q + |\vec{q}| \qquad\text{and}\qquad \omega_q - |\vec{q}| \leq \omega_p + |\vec{p}| \tag{6.16}$$

hold for all $|\vec{p}|,|\vec{q}|\geq 0$ which can be cast into the form $|\omega|\leq|k_+|$. Similarly, we find

$$\omega_p - |\vec{p}| \leq \omega_q - |\vec{q}| \quad\text{for } |\vec{p}|\geq|\vec{q}| \qquad\text{and}\qquad \omega_q - |\vec{q}| \leq \omega_p - |\vec{p}| \quad\text{for } |\vec{p}|\leq|\vec{q}| \tag{6.17}$$

which is equivalent to $|\omega| \leq |k_-|$. Taken together, we have $|\omega| \leq |k_\pm|$ which means that in the expressions for $I^{\bullet}_{\uparrow\downarrow|m}$ as derived in Lemma 6.1.6 only the lower cases are relevant for the evaluation of the above matrix. By considering, for example, the upper right entry of the matrix, we find

$$\begin{aligned}
&-\mathrm{i}\left[\frac{1}{|\vec{q}|}\big(I^{\cos}_{\downarrow|3}(\omega,k_+) - I^{\cos}_{\downarrow|3}(\omega,k_-)\big) + \big(I^{\sin}_{\downarrow|2}(\omega,k_+) + I^{\sin}_{\downarrow|2}(\omega,k_-)\big)\right] = \\
&= -\mathrm{i}\frac{\pi}{2}\left[\frac{\mathrm{i}\epsilon(\omega)|\omega||k_+| - \mathrm{i}\epsilon(\omega)|\omega||k_-|}{|\vec{q}|} + \big(\mathrm{i}\epsilon(-\omega)\epsilon(k_+)|\omega| + \mathrm{i}\epsilon(-\omega)\epsilon(k_-)|\omega|\big)\right] \\
&= \frac{\pi}{2}\omega\left[\frac{|k_+| - |k_-|}{|\vec{q}|} - \big(\epsilon(k_+) + \epsilon(k_-)\big)\right] \\
&= \frac{\pi}{2}\omega\begin{Bmatrix} \frac{|\vec{p}|+|\vec{q}|-(|\vec{p}|-|\vec{q}|)}{|\vec{q}|} - \big(1+1\big) & \text{for } |\vec{p}| \geq |\vec{q}| \\ \frac{|\vec{p}|+|\vec{q}|-(|\vec{q}|-|\vec{p}|)}{|\vec{q}|} - \big(1+(-1)\big) & \text{for } |\vec{p}| < |\vec{q}| \end{Bmatrix} = \pi \min\left\{\omega\frac{|\vec{p}|}{|\vec{q}|}, 0\right\} \qquad (6.18)
\end{aligned}$$

Evaluating all other entries in the same way, we finally end up with

$$\mathcal{F}\big[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}\big](|\vec{p}|,|\vec{q}|) = \frac{1/3}{(2\pi)^3}\frac{(c\varepsilon^d)^{-3}}{\omega_p\omega_q}\begin{pmatrix} -\min\left\{\frac{1}{|\vec{p}|},\frac{1}{|\vec{q}|}\right\} & \min\left\{0,\frac{|\vec{p}|}{|\vec{q}|^2}\frac{\omega_p-\omega_q}{|\vec{p}|}\right\} \\ \min\left\{0,\frac{|\vec{q}|}{|\vec{p}|^2}\frac{\omega_q-\omega_p}{|\vec{q}|}\right\} & -\frac{1}{3}\frac{\min\left\{\frac{|\vec{p}|^2}{|\vec{q}|},\frac{|\vec{q}|^2}{|\vec{p}|}\right\}}{|\vec{p}||\vec{q}|}\end{pmatrix}$$

which concludes the proof. □

6.2 Construction of the Inverse Operator for $\mathrm{S}^{\varepsilon}_{00}$

Having found an explicit expression for the angular-integrated incomplete Fourier transform $\mathcal{F}\big[\mathcal{N}^{\varepsilon}_{00|00}\big](|\vec{p}|,|\vec{q}|)$ without remaining position space integrals present, we are now in the position to construct the inverse operator of the term in the integral operator $\mathrm{S}^{\varepsilon}_{00}$ corresponding to $\mathcal{F}\big[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}\big](|\vec{p}|,|\vec{q}|)$. To this end, we recall that according to Theorem 4.3.1 the sesquilinear term in the l^{th} multipole moment of the second variation of the regularized causal action reads

$$\delta^2\mathcal{S}^{\varepsilon}_{\mathrm{sql},l} = \mathrm{Re}\left[\frac{1}{2}\sum_{m=-l}^{l}\left\langle\!\!\left\langle \Delta_{lm}, \mathrm{S}^{\varepsilon}_{lm}\Delta_{lm}\right\rangle\!\!\right\rangle\right]$$

where the integral operators $\mathrm{S}^{\varepsilon}_{lm}$ for $(l,m) \in \mathbb{N}_0 \times \mathbb{Z}$ with $-l \leq m \leq l$ are given by

$$\begin{aligned}(\mathrm{S}^{\varepsilon}_{lm}\Delta_{lm})(|\vec{p}|) \overset{(4.53b)}{=} \int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\Big[&\overline{\mathcal{F}\big[\mathcal{M}^{\varepsilon}_{lm|l(-m)}\big](|\vec{p}|,|\vec{q}|)} - \overline{\mathcal{F}\big[\mathcal{V}^{\varepsilon}_{lm|l(-m)}\big](|\vec{p}|,|\vec{q}|)} \\ &+ (-1)^{-m}\overline{\mathcal{F}\big[\mathcal{N}^{\varepsilon}_{lm|l(-m)}\big](|\vec{p}|,|\vec{q}|)} - (-1)^{-m}\overline{\mathcal{F}\big[\mathcal{W}^{\varepsilon}_{lm|l(-m)}\big](|\vec{p}|,|\vec{q}|)}\Big]\Delta_{lm}(|\vec{q}|)\end{aligned}$$

Due to the fact that, as already mentioned at the beginning of Subsection 6.1.1, the principal procedure is the same for all four terms in $\mathrm{S}^{\varepsilon}_{lm}$, we again restrict attention to the contribution coming from the incomplete Fourier transform $\mathcal{F}\big[\mathcal{N}^{\varepsilon}_{00|00}\big](|\vec{p}|,|\vec{q}|)$, or rather $\mathcal{F}\big[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}\big](|\vec{p}|,|\vec{q}|)$. Accordingly, the object of investigation in this section is

$$\delta^2\mathcal{S}^{\varepsilon}_{\mathrm{sql},0} = \mathrm{Re}\left[\frac{1}{2}\left\langle\!\!\left\langle \Delta_{00}\middle|\mathrm{S}^{\varepsilon,\mathrm{lc}}_{00}\Delta_{00}\right\rangle\!\!\right\rangle\right] \quad \text{where} \quad \mathrm{S}^{\varepsilon,\mathrm{lc}}_{00}\Delta_{00}(|\vec{p}|) = \int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\overline{\mathcal{F}\big[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}\big](|\vec{p}|,|\vec{q}|)}\Delta_{00}(|\vec{q}|)$$

As the entries of the matrix-valued integral kernel $\mathcal{F}[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}](|\vec{p}|,|\vec{q}|)$ vanish except for the upper left (2×2)-block matrix according to Lemma 6.1.7, we will suppress zero rows and columns in what follows and only consider two-component functions $\Delta_{00} \in C^\infty(\mathbb{R}^+_0,\mathbb{C}^2)$.

6.2.1 Construction of Green's Operators for Entries of $\mathcal{F}[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}]$

To begin with, we first construct differential operators which invert the diagonal entries of the matrix-valued integral kernel $\mathcal{F}\big[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}\big](|\vec{p}|,|\vec{q}|)$ in the sense of Green's operators.

LEMMA 6.2.1 (GREEN'S OPERATORS FOR DIAGONAL ENTRIES OF $\mathcal{F}[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}](|\vec{p}|,|\vec{q}|)$)

The non-vanishing diagonal entries

$$K_1(|\vec{p}|,|\vec{q}|) := \min\left\{\frac{1}{|\vec{p}|},\frac{1}{|\vec{q}|}\right\} \qquad \text{and} \qquad K_2(|\vec{p}|,|\vec{q}|) := \min\left\{\frac{|\vec{q}|^2}{|\vec{p}|},\frac{|\vec{p}|^2}{|\vec{q}|}\right\} \tag{6.19a}$$

of the matrix $\mathcal{F}\big[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}\big](|\vec{p}|,|\vec{q}|)$ as given in (6.15) are Green's functions of the differential operators

$$\mathrm{A} := -|\vec{p}|^2\left(\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}+\frac{2}{|\vec{p}|}\right)\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|} \qquad \text{and} \qquad \mathrm{B} := -\frac{1}{3}\left(\frac{\mathrm{d}^2}{\mathrm{d}|\vec{p}|^2}-\frac{2}{|\vec{p}|^2}\right) \tag{6.19b}$$

respectively.

Proof. In order to construct inverse operators for the non-vanishing diagonal entries of $\mathcal{F}\big[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}\big](|\vec{p}|,|\vec{q}|)$, we construct differential operators which have K_1 and K_2 as their Green's functions.

(1) Constructing the Green's Operator for K_1

From the form of K_1 we can immediately conclude that we need at least a second-order differential operator A (with respect to $|\vec{p}|$) in order to achieve that $\mathrm{A}K_1$ vanishes for $|\vec{p}|>|\vec{q}|$. Using the ansatz

$$\mathrm{A} = \alpha_2(|\vec{p}|)\frac{\mathrm{d}^2}{\mathrm{d}|\vec{p}|^2}+\frac{\alpha_1(|\vec{p}|)}{|\vec{p}|}\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}+\frac{\alpha_0(|\vec{p}|)}{|\vec{p}|^2}$$

and demanding that the condition

$$\mathrm{A}K_1(|\vec{p}|,|\vec{q}|) \overset{!}{=} 0$$

holds for $|\vec{p}|\neq|\vec{q}|$, we obtain the following restrictions on the choice of the coefficient functions $\alpha_0,\alpha_1,\alpha_2$ by considering the regions $|\vec{p}|<|\vec{q}|$ and $|\vec{p}|>|\vec{q}|$ separately

$$0 \overset{!}{=} \begin{cases} \alpha_0 & \text{for } |\vec{p}|<|\vec{q}| \\ 2\alpha_2-\alpha_1+\alpha_0 & \text{for } |\vec{p}|>|\vec{q}| \end{cases}$$

Setting $\alpha_0\equiv 0$ and choosing $\alpha_1\equiv 2\alpha_2$ we arrive at the intermediate result

$$\mathrm{A} = \alpha_2(|\vec{p}|)\left(\frac{\mathrm{d}^2}{\mathrm{d}|\vec{p}|^2}+\frac{2}{|\vec{p}|}\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\right)$$

In order to fix the so far undetermined function α_2, we integrate the defining condition $\mathrm{A}K_1(|\vec{p}|,|\vec{q}|)=\delta(|\vec{p}|-|\vec{q}|)$ over $\mathbb{R}^+_0$ and thus obtain

$$\int_0^\infty \mathrm{d}|\vec{p}|\;\alpha_2(|\vec{p}|)\left(\frac{\mathrm{d}^2}{\mathrm{d}|\vec{p}|^2}+\frac{2}{|\vec{p}|}\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\right)K_1(|\vec{p}|,|\vec{q}|) \overset{!}{=} 1$$

Integrating the first term by parts and exploiting that $\partial_{|\vec{p}|}K_1$ identically vanishes in the region $|\vec{p}|<|\vec{q}|$ results in

$$\int_{|\vec{q}|}^{\infty} \mathrm{d}|\vec{p}| \; \frac{\partial K_1(|\vec{p}|,|\vec{q}|)}{\partial|\vec{p}|}\left(- \frac{\mathrm{d}\alpha_2(|\vec{p}|)}{\mathrm{d}|\vec{p}|} + \frac{2\alpha_2(|\vec{p}|)}{|\vec{p}|}\right) + \lim_{|\vec{p}|\to\infty}\left(- \frac{\alpha_2(|\vec{p}|)}{|\vec{p}|^2}\right) \stackrel{!}{=} 1$$

By comparing the length dimensions on both sides of the equation we can immediately conclude that α_2 has to satisfy the condition $\dim(\alpha_2) = 2$. This observation directly leads to the choice $\alpha_2(|\vec{p}|) = -|\vec{p}|^2$ which not only makes the integrand vanish but also ensures that the boundary term converges to one. We conclude that the differential operator

$$\mathrm{A} = -|\vec{p}|^2\left(\frac{\mathrm{d}^2}{\mathrm{d}|\vec{p}|^2} + \frac{2}{|\vec{p}|}\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\right)$$

satisfies the condition

$$\mathrm{A}K_1(|\vec{p}|,|\vec{q}|) = \delta(|\vec{p}| - |\vec{q}|) \tag{6.20}$$

and is thus the sought-after Green's operator for K_1.

(2) Constructing the Green's Operator for K_2

In order to find a differential operator B which has K_2 as Green's function, we proceed in precisely the same way as above and again start from an ansatz for a second-order differential operator with respect to $|\vec{p}|$. By considering the regions $|\vec{p}| < |\vec{q}|$ and $|\vec{p}| > |\vec{q}|$ separately, we obtain the following conditions

$$0 \stackrel{!}{=} \begin{cases} 2(\beta_2 + \beta_1) + \beta_0 & \text{for } |\vec{p}| < |\vec{q}| \\ 2\beta_2 - \beta_1 + \beta_0 & \text{for } |\vec{p}| > |\vec{q}| \end{cases}$$

which implies $\beta_1 \equiv 0$ by taking the difference of the two conditions. Choosing $\beta_0 \equiv -2\beta_2$ we find

$$\mathrm{B} = \beta_2(|\vec{p}|)\left(\frac{\mathrm{d}^2}{\mathrm{d}|\vec{p}|^2} - \frac{2}{|\vec{p}|^2}\right)$$

In order to decide on how to choose the yet undetermined function β_2, we integrate the condition $\mathrm{B}K_2(|\vec{p}|,|\vec{q}|) = \delta(|\vec{p}| - |\vec{q}|)$ over $\mathbb{R}_0^+$ and thus obtain

$$\int_0^{\infty} \mathrm{d}|\vec{p}| \; \beta_2(|\vec{p}|)\left(\frac{\mathrm{d}^2}{\mathrm{d}|\vec{p}|^2} - \frac{2}{|\vec{p}|^2}\right)K_2(|\vec{p}|,|\vec{q}|) = 1$$

Integration by parts in the first term turns the condition into the form

$$\int_0^{\infty} \mathrm{d}|\vec{p}| \; \left(- \frac{\mathrm{d}\beta_2(|\vec{p}|)}{\mathrm{d}|\vec{p}|}\frac{\partial K_2(|\vec{p}|,|\vec{q}|)}{\partial|\vec{p}|} - \frac{2\beta_2(|\vec{p}|)}{|\vec{p}|^2}K_2(|\vec{p}|,|\vec{q}|)\right) + \left[\beta_2(|\vec{p}|)\frac{\partial K_2(|\vec{p}|,|\vec{q}|)}{\partial|\vec{p}|}\right]_0^{\infty} \stackrel{!}{=} 1$$

In contrast with the previous case, the partial derivative $\partial_{|\vec{p}|}K_2$ does not vanish for $|\vec{p}| < |\vec{q}|$. Splitting the integral into the regions $|\vec{p}| < |\vec{q}|$ and $|\vec{p}| > |\vec{q}|$ and inserting the respective expressions for the partial derivative $\partial_{|\vec{p}|}K_2$ leads to

$$\begin{aligned} &\frac{2}{|\vec{q}|}\left[\int_0^{|\vec{q}|} \mathrm{d}|\vec{p}| \; \left(- \beta_2(|\vec{p}|) - |\vec{p}|\frac{\mathrm{d}\beta_2(|\vec{p}|)}{\mathrm{d}|\vec{p}|}\right) - \lim_{|\vec{p}|\to 0} |\vec{p}|\beta_2(|\vec{p}|)\right] + \\ &+ |\vec{q}|^2\left[\int_{|\vec{q}|}^{\infty} \mathrm{d}|\vec{p}| \; \left(- \frac{2\beta_2(|\vec{p}|)}{|\vec{p}|^3} + \frac{1}{|\vec{p}|^2}\frac{\mathrm{d}\beta_2(|\vec{p}|)}{\mathrm{d}|\vec{p}|}\right) - \lim_{|\vec{p}|\to\infty}\frac{\beta_2(|\vec{p}|)}{|\vec{p}|^2}\right] \stackrel{!}{=} 1 \end{aligned}$$

From dimensional considerations we conclude that the function β_2 has to satisfy the condition $\dim(\beta_2) = 0$. By choosing $\beta_2(|\vec{p}|) = c \in \mathbb{R}$ and computing all integrals it remains

$$-\frac{2}{|\vec{q}|} \cdot c|\vec{q}| + |\vec{q}|^2 \cdot \left[\frac{c}{|\vec{p}|^2}\right]_{|\vec{q}|}^{\infty} \overset{!}{=} 1$$

which implies $c = -\frac{1}{3}$. As a consequence, the differential operator B has to be chosen as

$$\mathrm{B} = -\frac{1}{3}\left(\frac{\mathrm{d}^2}{\mathrm{d}|\vec{p}|^2} - \frac{2}{|\vec{p}|^2}\right)$$

in order for the Green's functions condition

$$\mathrm{B}K_2(|\vec{p}|, |\vec{q}|) = \delta(|\vec{p}| - |\vec{q}|) \tag{6.21}$$

to be satisfied. This concludes the proof. □

6.2.2 Differential Operator Representation of $\delta^2\mathcal{S}^{\varepsilon}_{\mathrm{sql},0}$

Having constructed the Green's operators for the non-vanishing diagonal entries of the matrix $\mathcal{F}[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}]$ we can now, in a second step, make use of these results by expressing the contribution to the multipole moment $\delta^2\mathcal{S}^{\varepsilon}_{\mathrm{sql},0}$ in (4.53b) corresponding to $\mathcal{F}[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}]$ in terms of a second-order differential operator with matrix potential.

Lemma 6.2.2 (Differential Operator Representation of $\delta^2\mathcal{S}^{\varepsilon}_{\mathrm{sql},0}$)

The contribution to the multipole moment $\delta^2\mathcal{S}^{\varepsilon}_{0}$ of the second variation of the regularized causal action corresponding to $\mathcal{F}[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}]$ can be expressed as

$$\delta^2\mathcal{S}^{\varepsilon}_{\mathrm{sql},0} = -\frac{(c\varepsilon^d)^{-3}}{24\pi^3}\,\mathrm{Re}\left[\frac{1}{2}\int_0^{\infty} \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^8}\,\Big\langle f(|\vec{p}|), \mathrm{H}f(|\vec{p}|)\Big\rangle_{\mathbb{C}^2}\right] \tag{6.22a}$$

where the differential operator H and the two-component function $f \in C^{\infty}(\mathbb{R}^+_0, \mathbb{C}^2)$ are given by

$$\mathrm{H} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}(-\Delta_{\mathbb{R}^3}) + \begin{pmatrix} 0 & -\frac{1}{2} \\ -\frac{1}{2} & 1 \end{pmatrix}\frac{1}{|\vec{p}|^2} \qquad \text{and} \qquad f = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} |\vec{p}|f_0 \\ |\vec{p}|f_1 \end{pmatrix} \tag{6.22b}$$

respectively.

Proof. According to the discussion at the beginning of Section 6.2, the contribution to the multipole moment $\delta^2\mathcal{S}^{\varepsilon}_{0}$ relevant for us is given by

$$\delta^2\mathcal{S}^{\varepsilon}_{\mathrm{sql},0} = \mathrm{Re}\left[\frac{1}{2}\left\langle\!\left\langle \Delta_{00}, \mathrm{S}^{\varepsilon,\mathrm{lc}}_{00}\Delta_{00}\right\rangle\!\right\rangle\right] \quad \text{with} \quad \mathrm{S}^{\varepsilon,\mathrm{lc}}_{00}\Delta_{00}(|\vec{p}|) = \int_0^{\infty}\frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\mathcal{F}\big[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}\big](|\vec{p}|, |\vec{q}|)\Delta_{00}(|\vec{q}|)$$

where the integral kernel reads

$$\mathcal{F}\big[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}\big](|\vec{p}|, |\vec{q}|) = \frac{1/3}{(2\pi)^3}\frac{(c\varepsilon^d)^{-3}}{\omega_p\omega_q}\begin{pmatrix} -\min\left\{\frac{1}{|\vec{p}|}, \frac{1}{|\vec{q}|}\right\} & \min\left\{0, \frac{|\vec{p}|}{|\vec{q}|^2}\frac{\omega_p-\omega_q}{|\vec{p}|}\right\} \\ \min\left\{0, \frac{|\vec{q}|}{|\vec{p}|^2}\frac{\omega_q-\omega_p}{|\vec{q}|}\right\} & -\frac{1}{3}\frac{\min\left\{\frac{|\vec{p}|^2}{|\vec{q}|}, \frac{|\vec{q}|^2}{|\vec{p}|}\right\}}{|\vec{p}||\vec{q}|} \end{pmatrix}$$

To keep the discussion as simple as possible, we slightly simplify the discussion by only considering the massless case $\mu = 0$ where $\omega_p = \sqrt{|\vec{p}|^2 + \mu^2}$ reduces to $|\vec{p}|$. This allows us to express the off-diagonal entries of the matrix in terms of the functions K_1 and K_2 from Lemma 6.2.1 as

$$\min\left\{0, \frac{|\vec{p}| - |\vec{q}|}{|\vec{q}|^2}\right\} \overset{(6.19a)}{=} -\left(\frac{1}{|\vec{p}|} - \frac{1}{|\vec{p}||\vec{q}|}\frac{|\vec{q}|^2}{|\vec{p}|}\right) = -\Theta(|\vec{q}| - |\vec{p}|)\left(K_1(|\vec{p}|, |\vec{q}|) - \frac{K_2(|\vec{p}|, |\vec{q}|)}{|\vec{p}||\vec{q}|}\right)$$
$$\min\left\{0, \frac{|\vec{q}| - |\vec{p}|}{|\vec{p}|^2}\right\} \overset{(6.19a)}{=} -\left(\frac{1}{|\vec{q}|} - \frac{1}{|\vec{p}||\vec{q}|}\frac{|\vec{p}|^2}{|\vec{q}|}\right) = -\Theta(|\vec{p}| - |\vec{q}|)\left(K_1(|\vec{p}|, |\vec{q}|) - \frac{K_2(|\vec{p}|, |\vec{q}|)}{|\vec{p}||\vec{q}|}\right)$$

and thus, in turn, makes it possible to cast the above integral kernel into the following symmetrized form

$$\mathcal{F}\big[\mathrm{N}^{\varepsilon,\mathrm{lc}}_{00|00}\big](|\vec{p}|, |\vec{q}|)\Big|_{\mu=0} \overset{(6.19a)}{=} \frac{1/3}{(2\pi)^3}\frac{(c\varepsilon^d)^{-3}}{|\vec{p}||\vec{q}|}\begin{pmatrix} -K_1(|\vec{p}|, |\vec{q}|) & -\frac{1}{2}\Big(K_1(|\vec{p}|, |\vec{q}|) - \frac{K_2(|\vec{p}|, |\vec{q}|)}{|\vec{p}||\vec{q}|}\Big) \\ -\frac{1}{2}\Big(K_1(|\vec{p}|, |\vec{q}|) - \frac{K_2(|\vec{p}|, |\vec{q}|)}{|\vec{p}||\vec{q}|}\Big) & -\frac{1}{3}\frac{K_2(|\vec{p}|, |\vec{q}|)}{|\vec{p}||\vec{q}|} \end{pmatrix}$$

Based on this form of the integral kernel we can now rewrite $\delta^2\mathcal{S}^{\varepsilon}_{\mathrm{sql},0}$ by using the Green's operators A, B derived in Lemma 6.2.1 in the following way: First, by exploiting that A and B are invertible operators, the functions $\Delta_{00} \in C^\infty(\mathbb{R}^+_0, \mathbb{C}^2)$ can be expressed as

$$\Delta_{00}(|\vec{p}|) = \begin{pmatrix} \mathrm{A}f_0(|\vec{p}|) \\ 3|\vec{p}|\mathrm{B}|\vec{p}|f_1(|\vec{p}|) \end{pmatrix} \tag{6.23}$$

where $f_0, f_1 \in C^\infty(\mathbb{R}^+_0, \mathbb{C})$ can be chosen arbitrarily. The appearance of additional factors $|\vec{p}|$ in the second component accounts for the fact that the length dimensions of K_1 and K_2 (and thus also the length dimensions of the differential operators A and B) differ by two.[a] In this way, we obtain

$$\delta^2\mathcal{S}^{\varepsilon}_{\mathrm{sql},0} = \frac{(c\varepsilon^d)^{-3}}{24\pi^3}\,\mathrm{Re}\Bigg[\frac{1}{2}\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|}{(2\pi)^4}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|}{(2\pi)^4} \times$$
$$\times \left\langle \begin{pmatrix} \mathrm{A}f_0(|\vec{p}|) \\ 3|\vec{p}|\mathrm{B}|\vec{p}|f_1(|\vec{p}|) \end{pmatrix}, \begin{pmatrix} -K_1 & -\frac{1}{2}\Big(K_1 - \frac{K_2}{|\vec{p}||\vec{q}|}\Big) \\ -\frac{1}{2}\Big(K_1 - \frac{K_2}{|\vec{p}||\vec{q}|}\Big) & -\frac{1}{3}\frac{K_2}{|\vec{p}||\vec{q}|} \end{pmatrix}\begin{pmatrix} \mathrm{A}f_0(|\vec{q}|) \\ 3|\vec{q}|\mathrm{B}|\vec{q}|f_1(|\vec{q}|) \end{pmatrix}\right\rangle_{\mathbb{C}^2}\Bigg]$$

where the prefactor $\frac{1}{|\vec{p}||\vec{q}|}$ has already been compensated by (part of) the integration measures. Now, by exploiting the fact that according to Lemma 6.2.1 the functions K_1 and K_2 are Green's functions of the differential operators A and B, respectively, they are inverses of the integral operators $T_1, T_2 : C^\infty(\mathbb{R}^+_0, \mathbb{C}) \to C^\infty(\mathbb{R}^+_0, \mathbb{C})$ defined as

$$(T_i f)(|\vec{p}|) := \int_0^\infty \mathrm{d}|\vec{q}|\;K_i(|\vec{p}|, |\vec{q}|)f(|\vec{q}|)$$

for $i = 1, 2$. The Green's operator A (with respect to $|\vec{p}|$, as indicated by the subscript), for example, then satisfies

$$\mathrm{A}_{|\vec{p}|}\big[(T_1 f)(|\vec{p}|)\big] = \int_0^\infty \mathrm{d}|\vec{q}|\;\mathrm{A}_{|\vec{p}|}K_1(|\vec{p}|, |\vec{q}|)f(|\vec{q}|) \overset{(6.20)}{=} \int_0^\infty \mathrm{d}|\vec{q}|\;\delta(|\vec{p}| - |\vec{q}|)f(|\vec{q}|) = f(|\vec{p}|)$$

and likewise for the Green's operator B. Using this, the above expression reduces to

$$\delta^2\mathcal{S}^{\varepsilon}_{\mathrm{sql},0} = \frac{(c\varepsilon^d)^{-3}}{24\pi^3}\,\mathrm{Re}\Bigg[\frac{1}{2}\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^8}\left\langle \begin{pmatrix} f_0(|\vec{p}|) \\ f_1(|\vec{p}|) \end{pmatrix}, \begin{pmatrix} -\mathrm{A} & -\frac{1}{2}(3|\vec{p}|\mathrm{B}|\vec{p}| - 3\mathrm{A}) \\ -\frac{1}{2}(3|\vec{p}|\mathrm{B}|\vec{p}| - 3\mathrm{A}) & -3|\vec{p}|\mathrm{B}|\vec{p}| \end{pmatrix}\begin{pmatrix} f_0(|\vec{p}|) \\ f_1(|\vec{p}|) \end{pmatrix}\right\rangle_{\mathbb{C}^2}\Bigg]$$

where we have already carried out the integral with respect to $|\vec{q}|$. As can be verified by a quick computation, the differential operators A and B are related via $3|\vec{p}|\mathrm{B}|\vec{p}| = \mathrm{A}+2$. Using this relation, we find that the integrand of the second variation of the regularized causal action now takes the form of a matrix-valued differential operator with matrix potential given by

$$\delta^2\mathcal{S}^\varepsilon_{\mathrm{sql},0} = \frac{(c\varepsilon^d)^{-3}}{24\pi^3}\,\mathrm{Re}\left[\frac{1}{2}\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^8}\left\langle \begin{pmatrix} f_0(|\vec{p}|) \\ f_1(|\vec{p}|)\end{pmatrix}, \left[\begin{pmatrix} -1 & 1 \\ 1 & -1\end{pmatrix}\mathrm{A} + \begin{pmatrix} 0 & -1 \\ -1 & -2\end{pmatrix}\right]\begin{pmatrix} f_0(|\vec{p}|) \\ f_1(|\vec{p}|)\end{pmatrix}\right\rangle_{\mathbb{C}^2}\right]$$

In order to turn this expression into the form as given in the statement, we perform a change of basis such that the first matrix becomes diagonal[b], rescale the functions f_0, f_1 as $|\vec{p}|f_i \to f_i$ and use that the differential operator A can be expressed in terms of the radial part of the Laplacian in $\mathbb{R}^3$ as $\mathrm{A} = -|\vec{p}|^2\Delta_{\mathbb{R}^3}$. In this way we finally end up with

$$\delta^2\mathcal{S}^\varepsilon_{\mathrm{sql},0} = -\frac{(c\varepsilon^d)^{-3}}{24\pi^3}\,\mathrm{Re}\left[\frac{1}{2}\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^8}\Big\langle f(|\vec{p}|), \mathrm{H}f(|\vec{p}|)\Big\rangle_{\mathbb{C}^2}\right] \overset{(4.52)}{=} -\frac{(c\varepsilon^d)^{-3}}{192\pi^7}\,\mathrm{Re}\left[\frac{1}{2}\langle\!\langle f, \mathrm{H}f\rangle\!\rangle\right]$$

where the differential operator H and the two-component function $f \in C^\infty(\mathbb{R}^+_0, \mathbb{C}^2)$ are given by

$$\mathrm{H} = \begin{pmatrix} 1 & 0 \\ 0 & 0\end{pmatrix}(-\Delta_{\mathbb{R}^3}) + \begin{pmatrix} 0 & -\frac{1}{2} \\ -\frac{1}{2} & 1\end{pmatrix}\frac{1}{|\vec{p}|^2} \qquad \text{and} \qquad f = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1\end{pmatrix}\begin{pmatrix} |\vec{p}|f_0 \\ |\vec{p}|f_1\end{pmatrix}$$

respectively.

This concludes the proof. □

[a] Recall that A and B are both second-order differential operators with the difference that A includes an additional factor $|\vec{p}|^2$ compared with B.

[b] The eigenvalues are $\lambda_1 = -2$ and $\lambda_2 = 0$ with the corresponding normalized eigenvectors being $v_1 = \frac{1}{\sqrt{2}}(1,-1)^{\mathrm{T}}$ and $v_2 = \frac{1}{\sqrt{2}}(1,1)^{\mathrm{T}}$, respectively

6.3 Invertibility of the Multipole Moment $\delta^2\mathcal{S}^\varepsilon_{\mathrm{sql},0}$

In this final section we now put together all previous results and demonstrate that the contribution $\delta^2\mathcal{S}^\varepsilon_{\mathrm{sql},0}$ to the multipole moment $\delta^2\mathcal{S}^\varepsilon_0$ is invertible. Due to the fact that the structure of the other incomplete Fourier transforms is not fundamentally different from $\mathcal{F}[\mathcal{N}^{\varepsilon,\mathrm{lc}}_{00|00}]$, the approach presented in this chapter can be transferred to also evaluate these other contributions. Although explicit calculations become increasingly lengthy, the procedure can in principle also be applied to higher-order multipole moments.

Lemma 6.3.1 (Estimate for the Matrix Potential)

For any $u = (u_1, u_2) \in \mathbb{C}^2$ and for $c \geq \frac{-1+\sqrt{2}}{\sqrt{2}}$ the following inequality holds

$$\left\langle \begin{pmatrix} u_1 \\ u_2\end{pmatrix}, \begin{pmatrix} 0 & -1/2 \\ -1/2 & 1\end{pmatrix}\begin{pmatrix} u_1 \\ u_2\end{pmatrix}\right\rangle_{\mathbb{C}^2} \geq -c\|u\|^2 \tag{6.24}$$

where $\|u\|^2 = |u_1|^2 + |u_2|^2$.

Proof. To prove the claimed inequality, we start by computing the scalar product

$$\left\langle \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \begin{pmatrix} 0 & -1/2 \\ -1/2 & 1 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \right\rangle_{\mathbb{C}^2} = |u_2|^2 - \mathrm{Re}\left(u_1 \overline{u_2}\right)$$

and subsequently demand that the inequality

$$|u_2|^2 - \mathrm{Re}\left(u_1\overline{u_2}\right) \geq -c\|u\|^2 \qquad \Leftrightarrow \qquad |u_2|^2 - \mathrm{Re}\left(u_1\overline{u_2}\right) + c\|u\|^2 \geq 0$$

holds for some $c > 0$. Making use of the standard inequality $\mathrm{Re}(z_1 z_2) \leq |z_1||z_2|$ which holds for arbitrary complex numbers $z_1, z_2 \in \mathbb{C}$, we find the following estimate

$$\begin{aligned} |u_2|^2 - \mathrm{Re}\left(u_1\overline{u_2}\right) + c\|u\|^2 &\geq c|u_1|^2 + (1+c)|u_2|^2 - |u_1||u_2| \\ &= c\left(|u_1|^2 - 2 \cdot \frac{1}{2c}|u_1||u_2|\right) + (1+c)|u_2|^2 \\ &= c\left(|u_1| - \frac{|u_2|}{2c}\right)^2 + |u_2|^2\left(1 + c - \frac{1}{4c}\right) \end{aligned}$$

where the first term, being the square of real numbers, is clearly non-negative. In order to ensure that also the second term is non-negative, the parameter $c > 0$ has to satisfy the condition

$$c \geq \frac{-1+\sqrt{2}}{2} \tag{6.25}$$

If this is condition is satisfied, the inequality

$$|u_2|^2 - \mathrm{Re}\left(u_1\overline{u_2}\right) + c\|u\|^2 \geq c|u_1|^2 + (1+c)|u_2|^2 - |u_1||u_2| \geq 0 \tag{6.26}$$

holds and thus concludes the proof. □

In addition to this estimate which allows to handle the matrix potential term in (6.22), we need a second inequality for the term containing the differential operator.

Lemma 6.3.2 (Inequality for the Scalar Hamiltonian)

For any compactly supported, complex-valued function $\psi \in C_0^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C})$ which vanishes in a neighbourhood of $0 \in \mathbb{R}^3$ the following inequality holds[82, Ch. 14]

$$\int_{\mathbb{R}^3} \mathrm{d}^3\vec{x}\ \left|\mathrm{grad}\,\psi(\vec{x})\right|^2 \geq \int_{\mathbb{R}^3} \mathrm{d}^3\vec{x}\ \frac{|\psi(\vec{x})|^2}{4r^2} \tag{6.27}$$

Proof. To prove the claimed relation, we follow the proof by John Baez[82, Ch. 14] and start from the relation

$$\mathrm{grad}\left(r^{1/2}\psi\right) = \frac{\vec{x}}{2r^{3/2}}\psi + r^{1/2}\,\mathrm{grad}\,\psi$$

where $r := |\vec{x}\,|$. Solving for the second term on the right-hand side and taking the square of the absolute value results in the following inequality for the gradient

$$\begin{aligned} \left|\mathrm{grad}\,\psi\right|^2 &= \left|\frac{\mathrm{grad}(r^{1/2}\psi)}{r^{1/2}} - \frac{\vec{x}}{2r^2}\psi\right|^2 \\ &= \frac{\left|\mathrm{grad}(r^{1/2}\psi)\right|^2}{r} - \frac{\mathrm{Re}\left(\vec{x}\cdot\mathrm{grad}(r^{1/2}\psi)\overline{\psi}\right)}{r^{5/2}} + \frac{|\psi|^2}{4r^2} \end{aligned}$$

$$\geq -\frac{1}{r^{3/2}} \operatorname{Re}\left(\frac{\partial\left(r^{1/2}\psi\right)}{\partial r}\overline{\psi}\right) + \frac{|\psi|^2}{4r^2}$$

which holds for any $r > 0$. Rewriting the first term as

$$\frac{1}{r^{3/2}} \operatorname{Re}\left(\frac{\partial\left(r^{1/2}\psi\right)}{\partial r}\overline{\psi}\right) = \frac{1}{2r^{3/2}}\left(\frac{|\psi|^2}{r^{1/2}} + r^{1/2}\frac{\partial\psi}{\partial r}\overline{\psi} + r^{1/2}\psi\frac{\partial\overline{\psi}}{\partial r}\right) = \frac{1}{2r^2}\frac{\partial(r|\psi|^2)}{\partial r}$$

and inserting the whole expression into the left-hand side of the claimed relation yields

$$\begin{aligned}\int_{\mathbb{R}^3} \mathrm{d}^3\vec{x}\ \left|\operatorname{grad}\psi(\vec{x})\right|^2 &\geq -\int_{\mathbb{R}^3} \mathrm{d}^3\vec{x}\ \frac{1}{r^{3/2}} \operatorname{Re}\left(\frac{\partial\left(r^{1/2}\psi\right)}{\partial r}\overline{\psi}\right) + \int_{\mathbb{R}^3} \mathrm{d}^3\vec{x}\ \frac{|\psi(\vec{x})|^2}{4r^2} \\ &= -\int_{\mathbb{R}^3} \mathrm{d}^3\vec{x}\ \frac{1}{2r^2}\frac{\partial(r|\psi|^2)}{\partial r} + \int_{\mathbb{R}^3} \mathrm{d}^3\vec{x}\ \frac{|\psi(\vec{x})|^2}{4r^2}\end{aligned}$$

Note that it is this point where we have to assume that the function ψ vanishes in a neighbourhood of $0 \in \mathbb{R}^3$ in order to be able to use the above inequality. Taking into account that in spherical coordinates the integration measure in the first integral yields a factor r^2, we actually have a boundary term with respect to the radial integral

$$\ldots = -\int_{S^2} \mathrm{d}\Omega\ \left[\frac{r|\psi|^2}{2}\right]_0^\infty + \int_{\mathbb{R}^3} \mathrm{d}^3\vec{x}\ \frac{|\psi(\vec{x})|^2}{4r^2}$$

As we only consider compactly supported functions, this boundary term vanishes not only at $r = 0$ but also for $r \to \infty$ such that we end up with the claimed relation

$$\int_{\mathbb{R}^3} \mathrm{d}^3\vec{x}\ \left|\operatorname{grad}\psi(\vec{x})\right|^2 \geq \int_{\mathbb{R}^3} \mathrm{d}^3\vec{x}\ \frac{|\psi(\vec{x})|^2}{4r^2} \tag{6.28}$$

which concludes the proof. □

Armed with the estimates from Lemma 6.3.1 and Lemma 6.3.2 we can now prove that the contribution $\delta^2\mathcal{S}^\varepsilon_{\mathrm{sql},0}$ to the second variation of the regularized causal action is invertible.

Theorem 6.3.3 (Invertibility of the Multipole Moment $\delta^2\mathcal{S}^\varepsilon_{\mathrm{sql},0}$)

The differential operator H from Lemma 6.2.2 which is given by

$$\mathrm{H} \overset{(6.22)}{=} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} (-\Delta_{\mathbb{R}^3}) + \begin{pmatrix} 0 & -\frac{1}{2} \\ -\frac{1}{2} & 1 \end{pmatrix} \frac{1}{|\vec{p}|^2} \tag{6.29}$$

satisfies the relation

$$\forall f \in C_0^\infty(\mathbb{R}^+ \setminus \{0\}, \mathbb{C}^2): \qquad \left\langle\!\!\left\langle f(|\vec{p}|), \mathrm{H}f(|\vec{p}|) \right\rangle\!\!\right\rangle > 0 \tag{6.30}$$

As a consequence, the contribution $\delta^2\mathcal{S}^\varepsilon_{\mathrm{sql},0}$ to the second variation of the regularized causal action as given in Lemma 6.2.2 is invertible on $C_0^\infty(\mathbb{R}^+ \setminus \{0\}, \mathbb{C}^2)$.

Proof. In order to prove the claimed inequality for the operator H, we start by inserting the definition of H along with the radial part of the Laplacian which is given by $\Delta_{\mathbb{R}^3} = |\vec{p}|^{-2}\partial_{|\vec{p}|}\left(|\vec{p}|^2\partial_{|\vec{p}|}\right)$ we find[a]

$$\left\langle\!\!\left\langle f(|\vec{p}|), \mathrm{H}f(|\vec{p}|) \right\rangle\!\!\right\rangle =$$

$$\overset{(4.52)}{=} \int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4} \left\langle f(|\vec{p}|), \mathrm{H}f(|\vec{p}|) \right\rangle_{\mathbb{C}^2}$$
$$= \int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4} \left\langle f(|\vec{p}|), \left[-\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix} \frac{1}{|\vec{p}|^2}\frac{\partial}{\partial|\vec{p}|}\left(|\vec{p}|^2 \frac{\partial f(|\vec{p}|)}{\partial|\vec{p}|}\right) + \begin{pmatrix}0 & -\frac{1}{2}\\ -\frac{1}{2} & 1\end{pmatrix} \frac{f(|\vec{p}|)}{|\vec{p}|^2}\right] \right\rangle_{\mathbb{C}^2}$$
$$= \int_0^\infty \frac{\mathrm{d}|\vec{p}|}{(2\pi)^4} \left\langle f(|\vec{p}|), \left[-\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix} \frac{\partial}{\partial|\vec{p}|}\left(|\vec{p}|^2 \frac{\partial f(|\vec{p}|)}{\partial|\vec{p}|}\right) + \begin{pmatrix}0 & -\frac{1}{2}\\ -\frac{1}{2} & 1\end{pmatrix} f(|\vec{p}|)\right] \right\rangle_{\mathbb{C}^2}$$

Integrating by parts in the first term and spelling out the scalar products in the resulting terms yields

$$\dots = \int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4} \left(\left|\frac{\partial f(|\vec{p}|)}{\partial|\vec{p}|}\right|^2 + \left\langle f(|\vec{p}|), \begin{pmatrix}0 & -\frac{1}{2}\\ -\frac{1}{2} & 1\end{pmatrix} \frac{f(|\vec{p}|)}{|\vec{p}|^2} \right\rangle_{\mathbb{C}^2} \right) - \left[\frac{|\vec{p}|^2 f(|\vec{p}|)}{(2\pi)^4} \frac{\overline{\partial f(|\vec{p}|)}}{\partial|\vec{p}|} \right]_0^\infty$$

As a consequence of the fact that the functions f are both compactly supported and vanish in a neighbourhood of the origin in $\mathbb{R}^3$, the boundary term vanishes identically. Making use of the inequalities from Lemma 6.3.1 and Lemma 6.3.2 for the first and second term, respectively, we end up with

$$\left\langle\!\!\left\langle f(|\vec{p}|), \mathrm{H}f(|\vec{p}|) \right\rangle\!\!\right\rangle \underset{(6.27)}{\overset{(6.24)}{\geq}} \int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4} \left(\frac{|f(|\vec{p}|)|^2}{4|\vec{p}|^2} - \frac{-1+\sqrt{2}}{2} \frac{|f(|\vec{p}|)|^2}{|\vec{p}|^2} \right)$$
$$= \frac{3-2\sqrt{2}}{4} \int_0^\infty \frac{\mathrm{d}|\vec{p}|}{(2\pi)^4} \, |f(|\vec{p}|)|^2 > 0$$

This concludes the proof that the differential operator H is positive and thus invertible. As the contribution $\delta^2\mathcal{S}^{\varepsilon}_{\mathrm{sql},0}$ to the second variation of the regularized causal action is proportional to $\langle\!\langle f(|\vec{p}|), \mathrm{H}f(|\vec{p}|)\rangle\!\rangle$ according to Lemma 6.2.2, we can conclude that $\delta^2\mathcal{S}^{\varepsilon}_{\mathrm{sql},0}$ is invertible on $C_0^\infty(\mathbb{R}^+ \setminus \{0\}, \mathbb{C}^2)$. □

[a] Note that the sesquilinear form as given in (4.52) is actually defined on functions taking values in $\mathbb{C}^5$. Due to our simplifications (see Lemma 6.1.7), however, it is sufficient to consider functions taking values in $\mathbb{C}^2$.

Part IV

Appendices

A

The Regularized Causal Lagrangian with iε-Regularization

Contents

In this appendix we derive various formulas for derivatives of the iε-regularized causal Lagrangian as introduced in (2.42).

A.1 Frequently Used Integral Transforms

We start by introducing basic Fourier sine and cosine integral transforms which are required to evaluate the iε-regularized kernel of the fermionic projector.

Lemma A.1.1 (Fourier Sine and Cosine Transforms)

Let $\alpha > 0$, $\mathrm{Re}(\beta) > 0$ and $\mathrm{Re}(\gamma) > 0$. Then, according to Erdélyi and Bateman, the Fourier sine transform of the functions $x\mathrm{e}^{-\beta\sqrt{x^2+\gamma^2}}$ and $(x^2+\gamma^2)^{-1/2}x\mathrm{e}^{-\beta\sqrt{x^2+\gamma^2}}$ are given by[83, p. 75, eqns. (35), (36)]

$$\int_0^\infty \mathrm{d}x\; x\sin(\alpha x)\mathrm{e}^{-\beta\sqrt{x^2+\gamma^2}} = \alpha\beta\gamma^2\frac{K_2\big(\gamma\sqrt{\alpha^2+\beta^2}\big)}{\alpha^2+\beta^2} \tag{A.1a}$$

$$\int_0^\infty \mathrm{d}x\; \frac{x\sin(\alpha x)}{\sqrt{x^2+\gamma^2}}\mathrm{e}^{-\beta\sqrt{x^2+\gamma^2}} = \alpha\gamma\frac{K_1\big(\gamma\sqrt{\alpha^2+\beta^2}\big)}{\sqrt{\alpha^2+\beta^2}} \tag{A.1b}$$

while the Fourier cosine transform of the functions $\mathrm{e}^{-\beta\sqrt{x^2+\gamma^2}}$ and $(x^2+\gamma^2)^{-1/2}\mathrm{e}^{-\beta\sqrt{x^2+\gamma^2}}$ evaluate to[83, p. 16/17, eqns. (26), (27)]

$$\int_0^\infty \mathrm{d}x\ \cos(\alpha x)\mathrm{e}^{-\beta\sqrt{x^2+\gamma^2}} = \beta\gamma\frac{K_1\big(\gamma\sqrt{\alpha^2+\beta^2}\big)}{\sqrt{\alpha^2+\beta^2}} \tag{A.2a}$$

$$\int_0^\infty \mathrm{d}x\ \frac{\cos(\alpha x)}{\sqrt{x^2+\gamma^2}}\mathrm{e}^{-\beta\sqrt{x^2+\gamma^2}} = K_0\big(\gamma\sqrt{\alpha^2+\beta^2}\big) \tag{A.2b}$$

where K_0, K_1, K_2 are referred to as the *modified Bessel functions of the second kind.*

Proof. See *Tables of Integral Transforms, Vol. I* by Erdélyi and Bateman.[83] □

A.2 Components of P^ε with iε-Regularization

In Lemma 2.3.3 we have derived the explicit expressions for the vector and scalar components g^ε_-, h^ε_- of the iε-regularized kernel of the fermionic projector. In preparation for Appendix Section A.3 where certain combinations of derivatives of the iε-regularized causal Lagrangian are calculated, we derive the derivatives of the components and re-express them in terms of the components of themselves. Before, however, we introduce the following definition.

Definition A.2.1 (Components of P^ε with iε-Regularization)

The vector and scalar components of the iε-regularized kernel of the fermionic projector (and its adjoint) are given in (2.37a), (2.37b) in terms of modified Bessel functions of the second kind, namely

$$g^\varepsilon_\mp(\xi) = \mp\mathrm{i}\frac{\mu^4}{(2\pi)^3}\frac{K_2(\Xi^\varepsilon_\mp)}{(\Xi^\varepsilon_\mp)^2} \tag{A.3}$$

$$h^\varepsilon_\mp(\xi) = \frac{\mu^3}{(2\pi)^3}\frac{K_1(\Xi^\varepsilon_\mp)}{\Xi^\varepsilon_\mp} \tag{A.4}$$

For convenience, we reinterpret $g^\varepsilon_\mp(\xi), h^\varepsilon_\mp(\xi)$ as functions $\tilde{g}_\mp, \tilde{h} : \mathbb{C} \to \mathbb{C}$ of the complex variable $\Xi^\varepsilon_\mp$ as

$$\tilde{g}_\mp(\Xi^\varepsilon_\mp) \coloneqq g^\varepsilon_\mp(\xi) \tag{A.5a}$$

$$\tilde{h}(\Xi^\varepsilon_\mp) \coloneqq h^\varepsilon_\mp(\xi) \tag{A.5b}$$

Lemma A.2.2 (Derivatives of the Components of P^ε with iε-Regularization)

The first and second derivatives of the component functions $g^\varepsilon_\mp, h^\varepsilon_\mp$ of the iε-regularized kernel of the fermionic projector as introduced in Definition A.2.1 evaluate to

$$\tilde{g}'_\mp = -\frac{1}{\Xi^\varepsilon_\mp}\Big(4\tilde{g}_\mp \mp \mathrm{i}\mu\tilde{h}\Big) \tag{A.6a}$$

$$\tilde{g}''_\mp = -5\frac{\tilde{g}'_\mp}{\Xi^\varepsilon_\mp} + \tilde{g}_\mp \tag{A.6b}$$

$$\tilde{h}' = \mp\mathrm{i}\frac{\Xi^\varepsilon_\mp}{\mu}\tilde{g}_\mp \tag{A.6c}$$

$$\tilde{h}'' = \mp\frac{\mathrm{i}}{\mu}\Big(\tilde{g}_\mp + \Xi^\varepsilon_\mp\tilde{g}'_\mp\Big) \tag{A.6d}$$

where we suppress the arguments. Note that the length dimensions of these derivatives (with respect to the dimensionless variable $\Xi^\varepsilon_\mp$) are the same as those of $\tilde{g}_\mp$ and $\tilde{h}$.

Proof. In order to compute the derivatives of the component functions $\tilde{g}_\mp$ and $\tilde{h}$, we use the following derivative[57, pp. 8.486/12] and recursion relation[57, 8.486/17] for modified Bessel functions

$$\frac{\mathrm{d}K_\nu(z)}{\mathrm{d}z} = -\Big(K_{\nu-1}(z) + \frac{\nu}{z}K_\nu(z)\Big) \quad \text{(A.7a)} \qquad K_2(z) = K_0(z) + 2\frac{K_1(z)}{z} \quad \text{(A.7b)}$$

Expressing the results in terms of $\tilde{g}_\mp$ and $\tilde{h}$ we obtain

$$\begin{aligned}\frac{\mathrm{d}\tilde{g}_\mp}{\mathrm{d}\Xi^\varepsilon_\mp} &\overset{\text{(A.7a)}}{=} \mp\mathrm{i}\frac{\mu^4}{(2\pi)^3}\Big(-4\frac{K_2(\Xi^\varepsilon_\mp)}{(\Xi^\varepsilon_\mp)^3} - \frac{K_1(\Xi^\varepsilon_\mp)}{(\Xi^\varepsilon_\mp)^2}\Big)\\ &= -\frac{1}{\Xi^\varepsilon_\mp}\Big(4\Big[\mp\mathrm{i}\frac{\mu^4}{(2\pi)^3}\frac{K_2(\Xi^\varepsilon_\mp)}{(\Xi^\varepsilon_\mp)^2}\Big] + \Big[\mp\mathrm{i}\frac{\mu^4}{(2\pi)^3}\frac{K_1(\Xi^\varepsilon_\mp)}{\Xi^\varepsilon_\mp}\Big]\Big) \overset{\text{(A.3)}}{\underset{\text{(A.5b)}}{=}} -\frac{1}{\Xi^\varepsilon_\mp}\Big(4\tilde{g}_\mp \mp \mathrm{i}\mu\tilde{h}\Big)\end{aligned} \tag{A.8}$$

$$\begin{aligned}\frac{\mathrm{d}\tilde{h}}{\mathrm{d}\Xi^\varepsilon_\mp} &\overset{\text{(A.7a)}}{=} \frac{\mu^3}{(2\pi)^3}\Big(-2\frac{K_1(\Xi^\varepsilon_\mp)}{(\Xi^\varepsilon_\mp)^2} - \frac{K_0(\Xi^\varepsilon_\mp)}{\Xi^\varepsilon_\mp}\Big)\\ &= -\frac{1}{\Xi^\varepsilon_\mp}\Big(\frac{\mu^3}{(2\pi)^3}\Big[2\frac{K_1(\Xi^\varepsilon_\mp)}{\Xi^\varepsilon_\mp} + K_0(\Xi^\varepsilon_\mp)\Big]\Big) \overset{\text{(A.5a)}}{\underset{\text{(A.7b)}}{=}} \mp\mathrm{i}\frac{\Xi^\varepsilon_\mp}{\mu}\tilde{g}_\mp\end{aligned} \tag{A.9}$$

Differentiating the above expressions once more and expressing the resulting expressions in terms of $\tilde{g}'_\mp$, $\tilde{g}_\mp$ and $\tilde{h}$ we find for the second derivatives

$$\begin{aligned}\frac{\mathrm{d}^2\tilde{g}_\mp}{\mathrm{d}(\Xi^\varepsilon_\mp)^2} &= \frac{1}{(\Xi^\varepsilon_\mp)^2}\Big(4\tilde{g}_\mp \mp \mathrm{i}\mu\tilde{h}\Big) - \frac{1}{\Xi^\varepsilon_\mp}\Big(4\tilde{g}'_\mp \mp \mathrm{i}\mu\tilde{h}'\Big)\\ &\overset{\text{(A.8)}}{\underset{\text{(A.9)}}{=}} -\frac{\tilde{g}'_\mp}{\Xi^\varepsilon_\mp} - \frac{1}{\Xi^\varepsilon_\mp}\Big(4\tilde{g}'_\mp \mp \mathrm{i}\mu\Big[\mp\mathrm{i}\frac{\Xi^\varepsilon_\mp}{\mu}\tilde{g}_\mp\Big]\Big) = -5\frac{\tilde{g}'_\mp}{\Xi^\varepsilon_\mp} + \tilde{g}_\mp\end{aligned} \tag{A.10}$$

$$\frac{\mathrm{d}^2\tilde{h}}{\mathrm{d}(\Xi^\varepsilon_\mp)^2} \overset{\text{(A.9)}}{=} \mp\mathrm{i}\frac{1}{\mu}\tilde{g}_\mp \mp \mathrm{i}\frac{\Xi^\varepsilon_\mp}{\mu}\tilde{g}'_\mp = \mp\frac{\mathrm{i}}{\mu}\Big(\tilde{g}_\mp + \Xi^\varepsilon_\mp\tilde{g}'_\mp\Big) \tag{A.11}$$

This concludes the proof. □

Corollary A.2.3 (Derivatives of Fourier Sine and Fourier Cosine Transforms)

Setting $\alpha \equiv r$, $\beta \equiv (\varepsilon \pm \mathrm{i}\xi^0)$ and $\gamma \equiv \mu$ in Lemma A.1.1, defining $\omega(x) := \sqrt{x^2+\mu^2}$ and expressing everything in terms of the functions $\tilde{g}_\mp, \tilde{h}$ as introduced in Definition A.2.1, we find the following relations

$$\int_0^\infty \frac{\mathrm{d}x}{(2\pi)^3}\begin{Bmatrix} x \\ x^3\end{Bmatrix}\frac{\sin(rx)}{\omega(x)}\mathrm{e}^{-(\varepsilon\pm\mathrm{i}\xi^0)\omega(x)} = \begin{Bmatrix} \frac{r}{\mu}\tilde{h} \\ \pm\mathrm{i}r\Big(3\tilde{g}_\mp + (\mu r)^2\frac{\tilde{g}'_\mp}{\Xi^\varepsilon_\mp}\Big)\end{Bmatrix} \tag{A.12a}$$

$$\int_0^\infty \frac{\mathrm{d}x}{(2\pi)^3}\begin{Bmatrix} x \\ x^3\end{Bmatrix}\sin(rx)\mathrm{e}^{-(\varepsilon\pm\mathrm{i}\xi^0)\omega(x)} = \begin{Bmatrix} -(\xi^\varepsilon_\mp)^0 r\tilde{g}_\mp \\ \mu^2(\xi^\varepsilon_\mp)^0 r\Big[3\frac{\tilde{g}'_\mp}{\Xi^\varepsilon_\mp} + \frac{(\mu r)^2}{(\Xi^\varepsilon_\mp)^2}\Big(\tilde{g}''_\mp - \frac{\tilde{g}'_\mp}{\Xi^\varepsilon_\mp}\Big)\Big]\end{Bmatrix} \tag{A.12b}$$

$$\int_0^\infty \frac{\mathrm{d}x}{(2\pi)^3}\, x\sin(rx)\omega(x)\mathrm{e}^{-(\varepsilon\pm\mathrm{i}\xi^0)\omega(x)} = \mp\mathrm{i}r\Big(\tilde{g}_\mp - \mu^2(\xi^\varepsilon_\mp)^0(\xi^\varepsilon_\mp)^0\frac{\tilde{g}'_\mp}{\Xi^\varepsilon_\mp}\Big) \tag{A.12c}$$

$$\int_0^\infty \frac{\mathrm{d}x}{(2\pi)^3} \begin{Bmatrix} x^2 \\ x^4 \end{Bmatrix} \frac{\cos(rx)}{\omega(x)} \mathrm{e}^{-(\varepsilon\pm\mathrm{i}\xi^0)\omega(x)} = \begin{Bmatrix} \frac{1}{\mu}\Big(\tilde{h} \mp \mathrm{i}\mu r^2 \tilde{g}_\mp\Big) \\ \pm\mathrm{i}\Big[3\tilde{g}_\mp + 6(\mu r)^2 \frac{\tilde{g}'_\mp}{\Xi^\varepsilon_\mp} + \frac{(\mu r)^4}{\Xi^\varepsilon_\mp}\Big(\tilde{g}''_\mp - \frac{\tilde{g}'_\mp}{\Xi^\varepsilon_\mp}\Big)\Big] \end{Bmatrix} \tag{A.12d}$$

$$\int_0^\infty \frac{\mathrm{d}x}{(2\pi)^3} x^2 \cos(rx) \mathrm{e}^{-(\varepsilon\pm\mathrm{i}\xi^0)\omega(x)} = -(\xi^\varepsilon_\mp)^0 \Big(\tilde{g}_\mp + (\mu r)^2 \frac{\tilde{g}'_\mp}{\Xi^\varepsilon_\mp}\Big) \tag{A.12e}$$

Proof. In order to derive the above relations, we set $\alpha \equiv r$, $\beta \equiv (\varepsilon \pm \mathrm{i}\xi^0)$ and $\gamma \equiv \mu$ in Lemma A.1.1 and thus find the following relation for $k \in \mathbb{N}_0$

$$\int_0^\infty \mathrm{d}x\ x^{2k+1} \sin(rx) \frac{\mathrm{e}^{-(\varepsilon\pm\mathrm{i}\xi^0)\omega(x)}}{\omega(x)} = \Big(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\Big)^k r\mu \frac{K_1\big(\mu\sqrt{r^2 + (\varepsilon \pm \mathrm{i}\xi^0)^2}\big)}{\sqrt{r^2 + (\varepsilon \pm \mathrm{i}\xi^0)^2}}$$

Expressing the right-hand side in terms of the dimensionless variable $\Xi^\varepsilon_\mp = \mu\sqrt{-(\xi^\varepsilon_\mp)^2}$ which can be rewritten as

$$(\xi^\varepsilon_\mp)^2 = (\xi^0 \mp \mathrm{i}\varepsilon)^2 - r^2 = -(\pm\mathrm{i})^2(\xi^0 \mp \mathrm{i}\varepsilon)^2 - r^2 = -\Big(r^2 + (\varepsilon \pm \mathrm{i}\xi^0)^2\Big)$$

and using the definition of the functions $\tilde{g}_\mp$ and $\tilde{h}$ as given in (A.5a) and (A.5b), respectively, we arrive at the central relation

$$\int_0^\infty \frac{\mathrm{d}x}{(2\pi)^3}\ x \sin(rx) \frac{\mathrm{e}^{-(\varepsilon\pm\mathrm{i}\xi^0)\omega(x)}}{\omega(x)} = \frac{r}{\mu}\tilde{h} \tag{A.13}$$

Starting from this we can now derive all other relations. By taking the j-fold derivative with respect to ξ^0 and the k-fold derivative with respect to r^2 and adjusting coefficients accordingly, we obtain

$$\int_0^\infty \frac{\mathrm{d}x}{(2\pi)^3}\ x^{2k+1} \sin(rx)\omega(x)^{j-1} \mathrm{e}^{-(\varepsilon\pm\mathrm{i}\xi^0)\omega(x)} = \Big(\pm\mathrm{i}\frac{\partial}{\partial\xi^0}\Big)^j \Big(-\frac{\partial^2}{\partial r^2}\Big)^k \frac{r}{\mu}\tilde{h}$$

The corresponding expressions (again for $k \in \mathbb{N}_0$) with sines replaced by cosines can be obtained from the above result by adding one derivative with respect to r

$$\int_0^\infty \frac{\mathrm{d}x}{(2\pi)^3}\ x^{2k+2} \cos(rx)\omega(x)^{j-1} \mathrm{e}^{-(\varepsilon\pm\mathrm{i}\xi^0)\omega(x)} = \frac{\mathrm{d}}{\mathrm{d}r}\Big(\pm\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\xi^0}\Big)^j \Big(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\Big)^k \frac{r}{\mu}\tilde{h}$$

Evaluating the expressions containing sines for $j = 0, 1, 2$ and $k = 0, 1$ and those containing cosines for $j = 0, 1$ and $k = 0$ by using the results from Lemma A.2.2 along with the relations

$$\frac{\partial \Xi^\varepsilon_\mp}{\partial \xi^0} = -\frac{\mu^2(\xi^\varepsilon_\mp)^0}{\Xi^\varepsilon_\mp} \qquad \frac{\partial \Xi^\varepsilon_\mp}{\partial r} = \frac{\mu^2 r}{\Xi^\varepsilon_\mp}$$

yields the claimed expressions and thus concludes the proof. □

With these relations at hand, we can now derive formulas for combined derivatives of the iε-regularized causal Lagrangian.

A.3 Derivatives of $\mathcal{L}^\varepsilon$ with iε-Regularization

Lemma A.3.1 (Derivatives of the Regularized Causal Lagrangian)

Let g, $\bar{g}$ and h, $\bar{h}$ be abbreviating notations defined as

$$g :- \tilde{g}_-(\Xi_-^\varepsilon) \qquad \text{(A.14a)} \qquad\qquad h :- \tilde{h}(\Xi_-^\varepsilon) \qquad \text{(A.14c)}$$

$$\bar{g} := \tilde{g}_+(\Xi_+^\varepsilon) \qquad \text{(A.14b)} \qquad\qquad \bar{h} := \tilde{h}(\Xi_+^\varepsilon) \qquad \text{(A.14d)}$$

and similarly for the derivatives. Then the first and second derivatives of the iε-regularized causal Lagrangian as given in (2.42) with respect to the differential operator $D := \partial_{\xi^0} + \frac{\xi^0}{r}\partial_r$ can be expressed as

$$\begin{aligned} D\mathcal{L}^\varepsilon(\xi) = 16(\varepsilon\mu)\,\mathrm{Re}\Bigg[&\mathrm{i}\mu\frac{g'}{\Xi_-^\varepsilon}\Big(B^\varepsilon|\xi^\varepsilon|^2\bar{g} - C^\varepsilon(\xi_-^\varepsilon)^2 g\Big) \\ &- \frac{\mathrm{i}}{\mu}g\Big(\big(B^\varepsilon\bar{g} - C^\varepsilon g\big) + \mathrm{i}\mu\big(B^\varepsilon\bar{h} + C^\varepsilon h\big)\Big)\Bigg] \end{aligned} \tag{A.15a}$$

$$\begin{aligned} D^2\mathcal{L}^\varepsilon(\xi) = 16(\varepsilon\mu)^2\,\mathrm{Re}\Bigg[&-\frac{\mu^2}{(\Xi_-^\varepsilon)^2}\Big(g'' - \frac{g'}{\Xi_-^\varepsilon}\Big)\Big(B^\varepsilon|\xi^\varepsilon|^2\bar{g} - C^\varepsilon(\xi_-^\varepsilon)^2 g\Big) \\ &- \mu^2\Big(\frac{g'}{\Xi_-^\varepsilon}\Big)^2\Big[\big(|\xi^\varepsilon|^2\big)^2\bar{g}^2 - C^\varepsilon(\xi_-^\varepsilon)^2\Big] \\ &- \mu^2\Big|\frac{g'}{\Xi_-^\varepsilon}\Big|^2\Big[-\big(|\xi^\varepsilon|^2\big)^2|g|^2 + 2(\xi_+^\varepsilon)^2(\xi_-^\varepsilon)^2|g|^2 - B^\varepsilon|\xi^\varepsilon|^2\Big] \\ &+ \frac{g'}{\Xi_-^\varepsilon}\Big[\mathrm{i}\mu\Big(2|g|^2\bar{h}|\xi^\varepsilon|^2 + 2\bar{g}^2 h|\xi^\varepsilon|^2 + 4|g|^2\bar{h}(\xi_-^\varepsilon)^2 + \big(B^\varepsilon\bar{h} + C^\varepsilon h\big)\Big) \\ &\qquad + 2\Big(2|g|^2\bar{g}(\xi_-^\varepsilon)^2 - C^\varepsilon g_-\Big) + \big(B^\varepsilon\bar{g} - C^\varepsilon g\big) - \big(B^\varepsilon\bar{g} + C^\varepsilon g\big)\Big] \\ &+ \frac{1}{\mu^2}\Big[-2\big(|g|^2\big)^2 - \mathrm{i}\mu|g|^2\Big(3g\bar{h} - \bar{g}h\Big) \\ &\qquad + \mu^2\Big(g^2\bar{h}^2 - |g|^2\big|h\big|^2 + g\big(B^\varepsilon\bar{g} + C^\varepsilon g\big)\Big)\Big]\Bigg] \end{aligned} \tag{A.15b}$$

where the functions B^ε and C^ε are those introduced in Definition 3.3.3.

Proof. In order to make the computation of $D\mathcal{L}^\varepsilon(\xi)$ and $D^2\mathcal{L}^\varepsilon(\xi)$ as simple and straightforward as possible, we first derive the expression for the first derivative of the functions $g_\mp$ and $h_\mp$ with respect to the differential operator $D := \partial_{\xi^0} + \frac{\xi^0}{r}\partial_r$ which yields

$$\begin{Bmatrix} D\tilde{g}_\mp \\ D\tilde{h} \end{Bmatrix} = \begin{Bmatrix} \frac{\mathrm{d}\tilde{g}_\mp}{\mathrm{d}\Xi_\mp^\varepsilon} \\ \frac{\mathrm{d}\tilde{h}}{\mathrm{d}\Xi_\mp^\varepsilon} \end{Bmatrix}\left(\frac{\partial\Xi_\mp^\varepsilon}{\partial\xi^0} + \frac{\xi^0}{r}\frac{\partial\Xi_\mp^\varepsilon}{\partial r}\right) \overset{\text{(A.6a)}}{\underset{\text{(A.6c)}}{=}} \pm\mathrm{i}\varepsilon\mu^2\begin{Bmatrix} \frac{\tilde{g}'_\mp}{\Xi_\mp^\varepsilon} \\ \mp\frac{\mathrm{i}}{\mu}\tilde{g}_\mp \end{Bmatrix} \tag{A.16}$$

Using these expressions we can now compute the first and second derivatives of $\mathcal{L}^\varepsilon(\xi)$ with respect to D.

(1) First Derivative of $\mathcal{L}^\varepsilon(\xi)$ with respect to $D := \partial_{\xi^0} + \frac{\xi^0}{r}\partial_r$
Acting with the differential operator D on the expression for the iε-regularized causal Lagrangian as given in (2.42) and using the above relations, we obtain

$$D\mathcal{L}(\xi^\varepsilon) = -16\varepsilon^2(Dr^2)(|g|^2)^2 - 64\varepsilon^2 r^2|g|^2\,\mathrm{Re}\left[\bar{g}Dg\right]$$

$$+8\,\mathrm{Re}\left[\big(D(\xi_-^\varepsilon)^2\big)g^2\bar{h}^2+2(\xi_-^\varepsilon)^2g(Dg)\bar{h}^2+2(\xi_-^\varepsilon)^2g^2\bar{h}(D\bar{h})\right]$$
$$+8\,\mathrm{Re}\left[\big(D|\xi^\varepsilon|^2\big)|g|^2|h|^2+2|\xi^\varepsilon|^2\,\mathrm{Re}\left[\bar{g}(Dg)\right]|h|^2+2|\xi^\varepsilon|^2|g|^2\,\mathrm{Re}\left[\bar{h}(Dh)\right]\right]$$

Using the relations $D|\xi^\varepsilon|^2=0$, $D(\xi_\mp^\varepsilon)=\mp 2\mathrm{i}\varepsilon$ and $Dr^2=2\xi^0$, the expression reduces to

$$\begin{aligned}\ldots=&-32\varepsilon^2\xi^0(|g|^2)^2-64\varepsilon^2r^2|g|^2\,\mathrm{Re}\left[\mathrm{i}\varepsilon\mu^2\bar{g}\frac{g'}{\Xi_-^\varepsilon}\right]\\&+8\,\mathrm{Re}\left[2\mathrm{i}\varepsilon g^2\bar{h}^2+2\mathrm{i}\varepsilon\mu^2(\xi_-^\varepsilon)^2g\frac{g'}{\Xi_-^\varepsilon}\bar{h}^2+2\varepsilon\mu(\xi_+^\varepsilon)^2\bar{g}^2hg\right]\\&+8\,\mathrm{Re}\left[2|\xi^\varepsilon|^2\,\mathrm{Re}\left[\mathrm{i}\varepsilon\mu^2\bar{g}\frac{g'}{\Xi_-^\varepsilon}\right]|h|^2+2\varepsilon\mu|\xi^\varepsilon|^2|g|^2\,\mathrm{Re}\left[g\bar{h}g\right]\right]\end{aligned}$$

where switched complex conjugations of the last term in the second line. Sorting terms according to their number of derivatives of g, we arrive at the following expression for $D\mathcal{L}^\varepsilon(\xi)$

$$\begin{aligned}\ldots=16(\varepsilon\mu)\,\mathrm{Re}\Bigg[&\mathrm{i}\mu\frac{g'}{\Xi_-^\varepsilon}\Big(-4\varepsilon^2r^2|g|^2\bar{g}+|\xi^\varepsilon|^2\bar{g}|h|^2+(\xi_-^\varepsilon)^2g\bar{h}^2\Big)\\&-\frac{\mathrm{i}}{\mu}\Big(g^2\bar{h}^2+\mathrm{i}\mu|g|^2\big((\xi_+^\varepsilon)^2\bar{g}h+|\xi^\varepsilon|^2g\bar{h}\big)-2\mathrm{i}\varepsilon\xi^0(|g|^2)^2\Big)\Bigg]\end{aligned}\tag{A.17}$$

Rewriting this result in terms of the functions B^ε and C^ε as introduced in Definition 3.3.3 we finally end up with

$$\begin{aligned}D\mathcal{L}^\varepsilon(\xi)&=16(\varepsilon\mu)\,\mathrm{Re}\Bigg[\mathrm{i}\mu\frac{g'}{\Xi_-^\varepsilon}\Big(B^\varepsilon|\xi^\varepsilon|^2\bar{g}-C^\varepsilon(\xi_-^\varepsilon)^2g\Big)\\&\qquad-\frac{\mathrm{i}}{\mu}\Big(\big(B^\varepsilon|g|^2-C^\varepsilon g^2\big)+\mathrm{i}\mu g\big(B^\varepsilon\bar{h}+C^\varepsilon h\big)-|g|^2\big(2\varepsilon^2|g|^2+|h|^2\big)\Big)\Bigg]\\&=16(\varepsilon\mu)\,\mathrm{Re}\Bigg[\mathrm{i}\mu\frac{g'}{\Xi_-^\varepsilon}\Big(B^\varepsilon|\xi^\varepsilon|^2\bar{g}-C^\varepsilon(\xi_-^\varepsilon)^2g\Big)\\&\qquad-\frac{\mathrm{i}}{\mu}g\Big(\big(B^\varepsilon\bar{g}-C^\varepsilon g\big)+\mathrm{i}\mu\big(B^\varepsilon\bar{h}+C^\varepsilon h\big)\Big)\Bigg]\end{aligned}\tag{A.18}$$

where in the final step we dropped the last term in the second line which vanishes as a consequence of the presence of the real part.

(2) Second Derivative of $\mathcal{L}^\varepsilon(\xi)$

For the computation of the second derivative of $\mathcal{L}^\varepsilon(\xi)$ with respect to D we take the expression for $D\mathcal{L}^\varepsilon(\xi)$ from (A.18) as our starting point. By acting with D on every term and using the relations $D|\xi^\varepsilon|^2=0$ and $D(\xi_\mp^\varepsilon)^2=\mp 2\mathrm{i}\varepsilon$ once more as well as $D\Xi_\mp^\varepsilon=\pm\mathrm{i}\varepsilon\frac{\mu^2}{\Xi_\mp^\varepsilon}$ we obtain

$$\begin{aligned}D^2\mathcal{L}^\varepsilon(\xi)=16(\varepsilon\mu)\,\mathrm{Re}\Bigg[&-\varepsilon\mu\frac{\mu^2}{(\Xi_-^\varepsilon)^2}\left(g''-\frac{g'}{\Xi_-^\varepsilon}\right)\Big(B^\varepsilon|\xi^\varepsilon|^2\bar{g}-C^\varepsilon(\xi_-^\varepsilon)^2g\Big)\\&+\mathrm{i}\mu\frac{g'}{\Xi_-^\varepsilon}\Big(DB^\varepsilon|\xi^\varepsilon|^2\bar{g}+B^\varepsilon|\xi^\varepsilon|^2D\bar{g}\\&\qquad-DC^\varepsilon(\xi_-^\varepsilon)^2g+2\mathrm{i}\varepsilon C^\varepsilon g-C^\varepsilon(\xi_-^\varepsilon)^2Dg\Big)\\&-\frac{\mathrm{i}}{\mu}Dg\Big(\big(B^\varepsilon\bar{g}-C^\varepsilon g\big)+\mathrm{i}\mu\big(B^\varepsilon\bar{h}+C^\varepsilon h\big)\Big)\\&-\frac{\mathrm{i}}{\mu}g\Big(\big(DB^\varepsilon\bar{g}+B^\varepsilon D\bar{g}-DC^\varepsilon g-C^\varepsilon Dg\big)\\&\qquad+\mathrm{i}\mu\big(DB^\varepsilon\bar{h}+B^\varepsilon D\bar{h}+DC^\varepsilon h+C^\varepsilon Dh\big)\Big)\Bigg]\end{aligned}$$

By making use of the derivatives of $\tilde{g}_\mp$ and $\tilde{h}$ we find for DB^ε and DC^ε the following relations

$$\begin{aligned} DB^\varepsilon &= 2(\varepsilon\mu)\Big(|\xi^\varepsilon|^2 \operatorname{Re}\Big[\mathrm{i}\mu\bar{g}\frac{g'}{\Xi_-^\varepsilon}\Big] + \operatorname{Re}\big[g\bar{h}\big]\Big) \\ DC^\varepsilon &= 2(\varepsilon\mu)\Big(\frac{\mathrm{i}}{\mu}\bar{g}^2 - \mathrm{i}\mu(\xi_+^\varepsilon)^2\bar{g}\frac{\bar{g}'}{\Xi_+^\varepsilon} - \bar{g}\bar{h}\Big) \end{aligned}$$

Inserting this into the above expression for $D^2\mathcal{L}^\varepsilon(\xi)$, simplifying the resulting expression and sorting terms according to their number of derivatives gives

$$\begin{aligned} \ldots = 16(\varepsilon\mu)^2 \operatorname{Re}\Bigg[&- \frac{\mu^2}{(\Xi_-^\varepsilon)^2}\Big(g'' - \frac{g'}{\Xi_-^\varepsilon}\Big)\Big(B^\varepsilon|\xi^\varepsilon|^2\bar{g} - C^\varepsilon(\xi_-^\varepsilon)^2 g\Big) \\ &- \mu^2\Big(\frac{g'}{\Xi_-^\varepsilon}\Big)^2\Big[\big(|\xi^\varepsilon|^2\big)^2\bar{g}^2 - C^\varepsilon(\xi_-^\varepsilon)^2\Big] \\ &- \mu^2\Big|\frac{g'}{\Xi_-^\varepsilon}\Big|^2\Big[-\big(|\xi^\varepsilon|^2\big)^2|g|^2 + 2(\xi_+^\varepsilon)^2(\xi_-^\varepsilon)^2|g|^2 - B^\varepsilon|\xi^\varepsilon|^2\Big] \\ &+ \frac{g'}{\Xi_-^\varepsilon}\Big[\mathrm{i}\mu\Big(2|g|^2\bar{h}|\xi^\varepsilon|^2 + 2\bar{g}^2 h|\xi^\varepsilon|^2 + 4|g|^2\bar{h}(\xi_-^\varepsilon)^2 + \big(B^\varepsilon\bar{h} + C^\varepsilon h\big)\Big) \\ &\qquad + 2\Big(2|g|^2\bar{g}(\xi_-^\varepsilon)^2 - C^\varepsilon g\Big) + \big(B^\varepsilon\bar{g} - C^\varepsilon g\big) - \big(B^\varepsilon\bar{g} + C^\varepsilon g\big)\Big] \\ &+ \frac{1}{\mu^2}\Big[-2\big(|g|^2\big)^2 - \mathrm{i}\mu|g|^2\Big(3g\bar{h} - \bar{g}h\Big) \\ &\qquad + \mu^2\Big(g^2\bar{h}^2 - |g|^2\big|h\big|^2 + g\big(B^\varepsilon\bar{g} + C^\varepsilon g\big)\Big)\Big]\Bigg] \end{aligned} \tag{A.19}$$

This concludes the proof. □

A.4 Light-Cone Expansions

LEMMA A.4.1 (LEADING-ORDER CONTRIBUTIONS OF THE COMPONENTS OF P^ε)

The leading-order singularities of $\tilde{g}_\mp(\Xi_\mp^\varepsilon)$ and $\tilde{h}(\Xi_\mp^\varepsilon)$ are given by

$$\tilde{g}_\mp(\Xi_\mp^\varepsilon) \mathrel{\mathring{=}} \mp\mathrm{i}\frac{2\mu^4}{(2\pi)^3}\frac{1}{(\Xi_\mp^\varepsilon)^4} \tag{A.20a}$$

$$\tilde{h}(\Xi_\mp^\varepsilon) \mathrel{\mathring{=}} \frac{\mu^3}{(2\pi)^3}\frac{1}{(\Xi_\mp^\varepsilon)^2} \tag{A.20b}$$

respectively.

Proof. Making use of the power series expansion of the modified Bessel functions $K_n(z)$ for $n \in \mathbb{N}_0$ around $z = 0$ which is given by[57, pp. 8.445, 8.446]

$$\begin{aligned} K_n(z) = \frac{1}{2}\Big(\frac{z}{2}\Big)^{-n}\sum_{k=0}^{n-1}\frac{(n-k-1)!}{k!}\Big(-\frac{z^2}{4}\Big)^k + (-1)^{n+1}\ln\Big(\frac{z}{2}\Big)I_n(z) \\ + (-1)^n\frac{1}{2}\Big(\frac{z}{2}\Big)^n\sum_{k=0}^{\infty}\frac{\psi(k+1)+\psi(n+k+1)}{k!(n+k)!}\Big(\frac{z}{2}\Big)^{2k} \end{aligned} \tag{A.21a}$$

where the functions ψ and I_n are defined in terms of the Γ-function as

$$\psi(z) = \frac{\Gamma'(z)}{\Gamma(z)} \qquad \text{and} \qquad I_n(z) = \left(\frac{z}{2}\right)^n \sum_{k=0}^{\infty} \frac{\left(\frac{z}{2}\right)^{2k}}{k!\Gamma(n+k+1)} \tag{A.21b}$$

As can be easily seen, the leading singularity of $K_n(z)$ for $n \geq 1$ is given by

$$K_n(z) \overset{\circ}{=} \frac{2^{n-1}}{z^n} \tag{A.22}$$

Applying this result to the functions $\tilde{g}_{\mp}(\Xi^{\varepsilon}_{\mp})$ and $\tilde{h}(\Xi^{\varepsilon}_{\mp})$ as introduced in (A.5a) and (A.5b), respectively, we thus find

$$\tilde{g}_{\mp}(\Xi^{\varepsilon}_{\mp}) \overset{\circ}{=} \mp\mathrm{i}\frac{2\mu^4}{(2\pi)^3}\frac{1}{(\Xi^{\varepsilon}_{\mp})^4} \qquad \text{and} \qquad \tilde{h}(\Xi^{\varepsilon}_{\mp}) \overset{\circ}{=} \frac{\mu^3}{(2\pi)^3}\frac{1}{(\Xi^{\varepsilon}_{\mp})^2} \tag{A.23}$$

□

B

Second Variation of the Eigenvalues of the Regularized Closed Chain

Contents

In this appendix we give the detailed calculations required in order to arrive at the expression (3.22b) in Lemma 3.3.7 for the second variation of the eigenvalues of the regularized closed chain which is, via the variation of the regularized causal Lagrangian as an intermediate step, one of the central ingredients in the computation of the variation of the regularized causal action.

B.1 Trace Identities for Commutators of Dirac Matrices

We start by deriving trace identities for products of up to four commutators of Dirac matrices which are needed to evaluate the second term in the general expression (3.23b) for the second variation of the eigenvalues of the regularized closed chain.

B.1.1 Trace Identities involving two Dirac Matrices

Proposition B.1.1 (Trace Identities involving to Dirac Matrices)

For two Dirac matrices we have the following two identities

$$\mathrm{Tr}\left[\gamma^i\gamma^j\right] = 4\eta^{ij} \qquad \text{(B.1a)} \qquad\qquad \mathrm{Tr}\left[[\gamma^i,\gamma^j]\right] = 0 \qquad \text{(B.1b)}$$

Proof. To prove the first identity, we split the expression into two parts, exploit the cyclicity of the trace and make use of $\{\gamma^i, \gamma^j\} = 2\eta^{ij}\mathrm{id}_{\mathbb{C}^4}$ which thus results in

$$\mathrm{Tr}\left[\gamma^i\gamma^j\right] = \frac{1}{2}\,\mathrm{Tr}\left[\gamma^i\gamma^j\right] + \frac{1}{2}\,\mathrm{Tr}\left[\gamma^j\gamma^i\right] = \frac{1}{2}\,\mathrm{Tr}\left[\{\gamma^i,\gamma^j\}\right] = \eta^{ij}\,\mathrm{Tr}\left[\mathrm{id}_{\mathbb{C}^4}\right] = 4\eta^{ij} \tag{B.2}$$

For the second identity we make use of the relation $[\gamma^i, \gamma^j] = 2(\gamma^i\gamma^j - \eta^{ij}\mathrm{id}_{\mathbb{C}^4})$ resulting from $\gamma^i\gamma^j = \frac{1}{2}[\gamma^i,\gamma^j] + \frac{1}{2}\{\gamma^i,\gamma^j\} = \frac{1}{2}[\gamma^i,\gamma^j] + \eta^{ij}\mathrm{id}_{\mathbb{C}^4}$. Along with the above result we find

$$\mathrm{Tr}\left[[\gamma^i,\gamma^j]\right] = 2\,\mathrm{Tr}\left[\gamma^i\gamma^j - \eta^{ij}\mathrm{id}_{\mathbb{C}^4}\right] = 2\Big\{\,\mathrm{Tr}\left[\gamma^i\gamma^j\right] - \eta^{ij}\,\mathrm{Tr}\left[\mathrm{id}_{\mathbb{C}^4}\right]\Big\} \overset{(B.2)}{=} 2\Big\{4\eta^{ij} - 4\eta^{ij}\Big\} = 0$$

This concludes the proof. □

B.1.2 Trace Identities involving four Dirac Matrices

In the case where there are four Dirac matrices, we have three trace identities corresponding to the number of possible commutators.

Proposition B.1.2 (Trace Identities involving Four Dirac Matrices)

For four Dirac matrices we have the following three identities

$$\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\right] = 4\big(\eta^{ij}\eta^{kl} - \eta^{ik}\eta^{jl} + \eta^{il}\eta^{jk}\big) \tag{B.3a}$$
$$\mathrm{Tr}\left[\gamma^i\gamma^j[\gamma^k,\gamma^l]\right] = 8\big(-\eta^{ik}\eta^{jl} + \eta^{il}\eta^{jk}\big) \tag{B.3b}$$
$$\mathrm{Tr}\left[[\gamma^i,\gamma^j][\gamma^k,\gamma^l]\right] = 16\big(-\eta^{ik}\eta^{jl} + \eta^{il}\eta^{jk}\big) \tag{B.3c}$$

Proof. To prove the first identity we make use of the relation $\gamma^i\gamma^j = 2\eta^{ij}\mathrm{id}_{\mathbb{C}^4} - \gamma^j\gamma^i$ resulting from $\{\gamma^i,\gamma^j\} = 2\eta^{ij}\mathrm{id}_{\mathbb{C}^4}$. In this way we find

$$\begin{aligned}
\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\right] &= \mathrm{Tr}\left[(2\eta^{ij} - \gamma^j\gamma^i)\gamma^k\gamma^l\right] \\
&= 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\right] - \mathrm{Tr}\left[\gamma^j(2\eta^{ik} - \gamma^k\gamma^i)\gamma^l\right] \\
&= 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\right] - 2\eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\right] + \mathrm{Tr}\left[\gamma^j\gamma^k(2\eta^{il} - \gamma^l\gamma^i)\right] \\
&= 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\right] - 2\eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\right] + 2\eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\right] - \mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^i\right]
\end{aligned} \tag{B.4}$$

By exploiting the cyclicity of the trace, the last term can be combined with the left-hand side which thus, together with (B.1a), results in

$$\begin{aligned}
\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\right] &= \eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\right] - \eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\right] + \eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\right] \\
&\overset{(B.1a)}{=} 4\big(\eta^{ij}\eta^{kl} - \eta^{ik}\eta^{jl} + \eta^{il}\eta^{jk}\big)
\end{aligned} \tag{B.5}$$

For the second identity we make use of the relation $[\gamma^k,\gamma^l] = 2(\gamma^k\gamma^l - \eta^{kl}\mathrm{id}_{\mathbb{C}^4})$ resulting from $\gamma^k\gamma^l = \frac{1}{2}[\gamma^k,\gamma^l] + \frac{1}{2}\{\gamma^k,\gamma^l\} = \frac{1}{2}[\gamma^k,\gamma^l] + \eta^{kl}\mathrm{id}_{\mathbb{C}^4}$. Along with the above result we find

$$\begin{aligned}
\mathrm{Tr}\left[\gamma^i\gamma^j[\gamma^k,\gamma^l]\right] &= 2\,\mathrm{Tr}\left[\gamma^i\gamma^j(\gamma^k\gamma^l - \eta^{kl})\right] \\
&= 2\Big\{\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\right] - \eta^{kl}\,\mathrm{Tr}\left[\gamma^i\gamma^j\right]\Big\} \\
&\overset{(B.5)}{=} 2\Big\{4\big(\cancelto{(1)}{\eta^{ij}\eta^{kl}} - \eta^{ik}\eta^{jl} + \eta^{il}\eta^{jk}\big) - \cancelto{(1)}{4\eta^{kl}\eta^{ij}}\Big\} \\
&= 8\big(-\eta^{ik}\eta^{jl} + \eta^{il}\eta^{jk}\big)
\end{aligned} \tag{B.6}$$

Finally, for the third identity we make repeated use of the relation $[\gamma^i, \gamma^j] = 2(\gamma^i\gamma^j - \eta^{ij}\mathrm{id}_{\mathbb{C}^4})$ resulting from $\gamma^i\gamma^j = \frac{1}{2}[\gamma^i, \gamma^j] + \frac{1}{2}\{\gamma^i, \gamma^j\} = \frac{1}{2}[\gamma^i, \gamma^j] + \eta^{ij}\mathrm{id}_{\mathbb{C}^4}$. Along with the results (B.1a) and (B.5) we find

$$\begin{aligned}
\mathrm{Tr}\left[[\gamma^i, \gamma^j][\gamma^k, \gamma^l]\right] &= 4\,\mathrm{Tr}\left[(\gamma^i\gamma^j - \eta^{ij}\mathrm{id}_{\mathbb{C}^4})(\gamma^k\gamma^l - \eta^{kl}\mathrm{id}_{\mathbb{C}^4})\right] \\
&= 4\Big\{\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\right] - \eta^{kl}\,\mathrm{Tr}\left[\gamma^i\gamma^j\right] - \eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\right] + \eta^{ij}\eta^{kl}\,\mathrm{Tr}\left[\mathrm{id}_{\mathbb{C}^4}\right]\Big\} \\
&\overset{(B.1a)}{\underset{(B.5)}{=}} 4\Big\{4\big(\cancel{\eta^{ij}\eta^{kl}}^{(1)} - \eta^{ik}\eta^{jl} + \eta^{il}\eta^{jk}\big) - \cancel{4\eta^{kl}\eta^{ij}}^{(1)} - \cancel{4\eta^{ij}\eta^{kl}}^{(2)} + \cancel{4\eta^{ij}\eta^{kl}}^{(2)}\Big\} \\
&= 16\big(-\eta^{ik}\eta^{jl} + \eta^{il}\eta^{jk}\big)
\end{aligned}$$

This concludes the proof. □

B.1.3 Trace Identities involving six Dirac Matrices

In the case where there are six Dirac matrices, the number of commutators no longer corresponds to the number of possible trace identities: While for zero, one and three commutators we can always arrange the commutators within the trace such that they appear at the last position, this is not possible if there are to commutators: Either the commutators are adjacent to each other (and thus can be commuted to the last position) or there is one Dirac matrix in between. All other possible positions (i. e. two Dirac matrices in between the commutators) can be recovered from those two standard cases by cyclic permutation and relabelling of the indices.

Proposition B.1.3 (Trace Identities involving Six Dirac Matrices)

For six Dirac matrices we have the following four identities which are relevant for the evaluation of the second term in (3.23b)

$$\begin{aligned}
&\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\right] = \\
&\quad = 4\Big\{\eta^{ij}\big(\eta^{kl}\eta^{mn} - \eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big) - \eta^{ik}\big(\eta^{jl}\eta^{mn} - \eta^{jm}\eta^{ln} + \eta^{jn}\eta^{lm}\big) \\
&\qquad + \eta^{il}\big(\eta^{jk}\eta^{mn} - \eta^{jm}\eta^{kn} + \eta^{jn}\eta^{km}\big) - \eta^{im}\big(\eta^{jk}\eta^{ln} - \eta^{jl}\eta^{kn} + \eta^{jn}\eta^{kl}\big) \\
&\qquad + \eta^{in}\big(\eta^{jk}\eta^{lm} - \eta^{jl}\eta^{km} + \eta^{jm}\eta^{kl}\big)\Big\}
\end{aligned} \tag{B.7a}$$

$$\begin{aligned}
&\mathrm{Tr}\left[\gamma^i\gamma^j[\gamma^k, \gamma^l][\gamma^m, \gamma^n]\right] = \\
&\quad = 16\Big\{\eta^{ij}\big(-\eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big) - \eta^{ik}\big(-\eta^{jm}\eta^{ln} + \eta^{jn}\eta^{lm}\big) \\
&\qquad + \eta^{il}\big(-\eta^{jm}\eta^{kn} + \eta^{jn}\eta^{km}\big) - \eta^{im}\big(\eta^{jk}\eta^{ln} - \eta^{jl}\eta^{kn}\big) \\
&\qquad + \eta^{in}\big(\eta^{jk}\eta^{lm} - \eta^{jl}\eta^{km}\big)\Big\}
\end{aligned} \tag{B.7b}$$

$$\begin{aligned}
&\mathrm{Tr}\left[\gamma^i[\gamma^j, \gamma^k]\gamma^l[\gamma^m, \gamma^n]\right] = \\
&\quad = 16\Big\{\eta^{ij}\big(-\eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big) - \eta^{ik}\big(-\eta^{jm}\eta^{ln} + \eta^{jn}\eta^{lm}\big) \\
&\qquad + \eta^{il}\big(-\eta^{jm}\eta^{kn} + \eta^{jn}\eta^{km}\big) - \eta^{im}\big(-\eta^{jl}\eta^{kn} + \eta^{jn}\eta^{kl}\big) \\
&\qquad + \eta^{in}\big(-\eta^{jl}\eta^{km} + \eta^{jm}\eta^{kl}\big)\Big\}
\end{aligned} \tag{B.7c}$$

$$\begin{aligned}
&\mathrm{Tr}\left[[\gamma^i, \gamma^j][\gamma^k, \gamma^l][\gamma^m, \gamma^n]\right] = \\
&\quad = 32\Big\{-\eta^{ik}\big(-\eta^{jm}\eta^{ln} + \eta^{jn}\eta^{lm}\big) + \eta^{il}\big(-\eta^{jm}\eta^{kn} + \eta^{jn}\eta^{km}\big) \\
&\qquad - \eta^{im}\big(\eta^{jk}\eta^{ln} - \eta^{jl}\eta^{kn}\big) + \eta^{in}\big(\eta^{jk}\eta^{lm} - \eta^{jl}\eta^{km}\big)\Big\}
\end{aligned} \tag{B.7d}$$

Proof. To prove the first identity, we make repeated use of the relation $\gamma^i\gamma^j = 2\eta^{ij}\mathrm{id}_{\mathbb{C}^4} - \gamma^j\gamma^i$ resulting from $\{\gamma^i,\gamma^j\} = 2\eta^{ij}\mathrm{id}_{\mathbb{C}^4}$. In this way we find

$$
\begin{aligned}
&\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\right] = \\
&\quad = \mathrm{Tr}\left[(2\eta^{ij}\mathrm{id}_{\mathbb{C}^4} - \gamma^j\gamma^i)\gamma^k\gamma^l\gamma^m\gamma^n\right] \\
&\quad = 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\right] - \mathrm{Tr}\left[\gamma^j(2\eta^{ik}\mathrm{id}_{\mathbb{C}^4} - \gamma^k\gamma^i)\gamma^l\gamma^m\gamma^n\right] \\
&\quad = 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\right] - 2\eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\right] + \mathrm{Tr}\left[\gamma^j\gamma^k(2\eta^{il}\mathrm{id}_{\mathbb{C}^4} - \gamma^l\gamma^i)\gamma^m\gamma^n\right] \\
&\quad = 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\right] - 2\eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\right] + 2\eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^m\gamma^n\right] \\
&\qquad\qquad - \mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l(2\eta^{im}\mathrm{id}_{\mathbb{C}^4} - \gamma^m\gamma^i)\gamma^n\right] \\
&\quad = 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\right] - 2\eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\right] + 2\eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^m\gamma^n\right] \\
&\qquad - 2\eta^{im}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^n\right] + \mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m(2\eta^{in}\mathrm{id}_{\mathbb{C}^4} - \gamma^n\gamma^i)\right] \\
&\quad = 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\right] - 2\eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\right] + 2\eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^m\gamma^n\right] \\
&\qquad - 2\eta^{im}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^n\right] + 2\eta^{in}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\right] - \mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^i\right]
\end{aligned}
$$

By exploiting the cyclicity of the trace, the last term can be combined with the left-hand side which thus, together with (B.3a), yields

$$
\begin{aligned}
&\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\right] = \\
&\quad = \eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\right] - \eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\right] + \eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^m\gamma^n\right] \\
&\qquad\qquad - \eta^{im}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^n\right] + \eta^{in}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\right] \\
&\quad \overset{\text{(B.3a)}}{=} 4\eta^{ij}\left(\eta^{kl}\eta^{mn} - \eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\right) - 4\eta^{ik}\left(\eta^{jl}\eta^{mn} - \eta^{jm}\eta^{ln} + \eta^{jn}\eta^{lm}\right) \\
&\qquad + 4\eta^{il}\left(\eta^{jk}\eta^{mn} - \eta^{jm}\eta^{kn} + \eta^{jn}\eta^{km}\right) - 4\eta^{im}\left(\eta^{jk}\eta^{ln} - \eta^{jl}\eta^{kn} + \eta^{jn}\eta^{kl}\right) \\
&\qquad\qquad + 4\eta^{in}\left(\eta^{jk}\eta^{lm} - \eta^{jl}\eta^{km} + \eta^{jm}\eta^{kl}\right)
\end{aligned} \tag{B.8}
$$

For the second identity we again make repeated use of the relation $[\gamma^i,\gamma^j] = 2(\gamma^i\gamma^j - \eta^{ij}\mathrm{id}_{\mathbb{C}^4})$ resulting from $\gamma^i\gamma^j = \frac{1}{2}[\gamma^i,\gamma^j] + \frac{1}{2}\{\gamma^i,\gamma^j\} = \frac{1}{2}[\gamma^i,\gamma^j] + \eta^{ij}\mathrm{id}_{\mathbb{C}^4}$. In this way we find

$$
\begin{aligned}
&\mathrm{Tr}\left[\gamma^i\gamma^j[\gamma^k,\gamma^l][\gamma^m,\gamma^n]\right] = \\
&\quad = 4\,\mathrm{Tr}\left[\gamma^i\gamma^j(\gamma^k\gamma^l - \eta^{kl}\mathrm{id}_{\mathbb{C}^4})(\gamma^m\gamma^n - \eta^{mn}\mathrm{id}_{\mathbb{C}^4})\right] \\
&\quad = 4\Big\{\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\right] - \eta^{mn}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\right] - \eta^{kl}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^m\gamma^n\right] + \eta^{kl}\eta^{mn}\,\mathrm{Tr}\left[\gamma^i\gamma^j\right]\Big\} \\
&\quad \overset{\text{(B.3a)}}{\underset{\text{(B.7a)}}{=}} 4\Big\{4\eta^{ij}\left(\eta^{kl}\eta^{mn} - \eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\right) - 4\eta^{ik}\left(\eta^{jl}\eta^{mn} - \eta^{jm}\eta^{ln} + \eta^{jn}\eta^{lm}\right) \\
&\qquad + 4\eta^{il}\left(\eta^{jk}\eta^{mn} - \eta^{jm}\eta^{kn} + \eta^{jn}\eta^{km}\right) - 4\eta^{im}\left(\eta^{jk}\eta^{ln} - \eta^{jl}\eta^{kn} + \eta^{jn}\eta^{kl}\right) \\
&\qquad\quad + 4\eta^{in}\left(\eta^{jk}\eta^{lm} - \eta^{jl}\eta^{km} + \eta^{jm}\eta^{kl}\right) - 4\eta^{mn}\left(\eta^{ij}\eta^{kl} - \eta^{ik}\eta^{jl} + \eta^{il}\eta^{jk}\right) \\
&\qquad\qquad - 4\eta^{kl}\left(\eta^{ij}\eta^{mn} - \eta^{im}\eta^{jn} + \eta^{in}\eta^{jm}\right) + 4\eta^{kl}\eta^{mn}\eta^{ij}\Big\} \\
&\quad = 4\Big\{4\eta^{ij}\left(\cancelto{(1)}{\eta^{kl}\eta^{mn}} - \eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\right) - 4\eta^{ik}\left(\cancelto{(2)}{\eta^{jl}\eta^{mn}} - \eta^{jm}\eta^{ln} + \eta^{jn}\eta^{lm}\right) \\
&\qquad + 4\eta^{il}\left(\cancelto{(3)}{\eta^{jk}\eta^{mn}} - \eta^{jm}\eta^{kn} + \eta^{jn}\eta^{km}\right) - 4\eta^{im}\left(\eta^{jk}\eta^{ln} - \eta^{jl}\eta^{kn} + \cancelto{(4)}{\eta^{jn}\eta^{kl}}\right) \\
&\qquad\quad + 4\eta^{in}\left(\eta^{jk}\eta^{lm} - \eta^{jl}\eta^{km} + \cancelto{(5)}{\eta^{jm}\eta^{kl}}\right) - 4\eta^{mn}\left(\cancelto{(1)}{\eta^{ij}\eta^{kl}} - \cancelto{(2)}{\eta^{ik}\eta^{jl}} + \cancelto{(3)}{\eta^{il}\eta^{jk}}\right) \\
&\qquad\qquad - 4\eta^{kl}\left(\cancelto{(6)}{\eta^{ij}\eta^{mn}} - \cancelto{(4)}{\eta^{im}\eta^{jn}} + \cancelto{(5)}{\eta^{in}\eta^{jm}}\right) + \cancelto{(6)}{4\eta^{kl}\eta^{mn}\eta^{ij}}\Big\} \\
&\quad = 16\Big\{\eta^{ij}\left(-\eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\right) - \eta^{ik}\left(-\eta^{jm}\eta^{ln} + \eta^{jn}\eta^{lm}\right) + \eta^{il}\left(-\eta^{jm}\eta^{kn} + \eta^{jn}\eta^{km}\right) \\
&\qquad\qquad - \eta^{im}\left(\eta^{jk}\eta^{ln} - \eta^{jl}\eta^{kn}\right) + \eta^{in}\left(\eta^{jk}\eta^{lm} - \eta^{jl}\eta^{km}\right)\Big\}
\end{aligned}
$$

For the third identity we once more make repeated use of the relation $[\gamma^i,\gamma^j] = 2(\gamma^i\gamma^j - \eta^{ij}\mathrm{id}_{\mathbb{C}^4})$ resulting from $\gamma^i\gamma^j = \frac{1}{2}[\gamma^i,\gamma^j] + \frac{1}{2}\{\gamma^i,\gamma^j\} = \frac{1}{2}[\gamma^i,\gamma^j] + \eta^{ij}\mathrm{id}_{\mathbb{C}^4}$. In this way we find

$$
\begin{aligned}
&\mathrm{Tr}\left[\gamma^i[\gamma^j,\gamma^k]\gamma^l[\gamma^m,\gamma^n]\right] = \\
&\quad = 4\,\mathrm{Tr}\left[\gamma^i(\gamma^j\gamma^k - \eta^{jk}\mathrm{id}_{\mathbb{C}^4})\gamma^l(\gamma^m\gamma^n - \eta^{mn}\mathrm{id}_{\mathbb{C}^4})\right] \\
&\quad = 4\Big\{\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\right] - \eta^{mn}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\right] - \eta^{jk}\,\mathrm{Tr}\left[\gamma^i\gamma^l\gamma^m\gamma^n\right] + \eta^{jk}\eta^{mn}\,\mathrm{Tr}\left[\gamma^i\gamma^l\right]\Big\} \\
&\quad \overset{\text{(B.3a)}}{\underset{\text{(B.7a)}}{=}} 4\Big\{4\eta^{ij}\big(\eta^{kl}\eta^{mn} - \eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big) - 4\eta^{ik}\big(\eta^{jl}\eta^{mn} - \eta^{jm}\eta^{ln} + \eta^{jn}\eta^{lm}\big) \\
&\qquad + 4\eta^{il}\big(\eta^{jk}\eta^{mn} - \eta^{jm}\eta^{kn} + \eta^{jn}\eta^{km}\big) - 4\eta^{im}\big(\eta^{jk}\eta^{ln} - \eta^{jl}\eta^{kn} + \eta^{jn}\eta^{kl}\big) \\
&\qquad + 4\eta^{in}\big(\eta^{jk}\eta^{lm} - \eta^{jl}\eta^{km} + \eta^{jm}\eta^{kl}\big) - 4\eta^{mn}\big(\eta^{ij}\eta^{kl} - \eta^{ik}\eta^{jl} + \eta^{il}\eta^{jk}\big) \\
&\qquad - 4\eta^{jk}\big(\eta^{il}\eta^{mn} - \eta^{im}\eta^{ln} + \eta^{in}\eta^{lm}\big) + 4\eta^{jk}\eta^{mn}\eta^{il}\Big\} \\
&\quad = 4\Big\{4\eta^{ij}\big(\cancelto{(1)}{\eta^{kl}\eta^{mn}} - \eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big) - 4\eta^{ik}\big(\cancelto{(2)}{\eta^{jl}\eta^{mn}} - \eta^{jm}\eta^{ln} + \eta^{jn}\eta^{lm}\big) \\
&\qquad + 4\eta^{il}\big(\cancelto{(3)}{\eta^{jk}\eta^{mn}} - \eta^{jm}\eta^{kn} + \eta^{jn}\eta^{km}\big) - 4\eta^{im}\big(\cancelto{(4)}{\eta^{jk}\eta^{ln}} - \eta^{jl}\eta^{kn} + \eta^{jn}\eta^{kl}\big) \\
&\qquad + 4\eta^{in}\big(\cancelto{(5)}{\eta^{jk}\eta^{lm}} - \eta^{jl}\eta^{km} + \eta^{jm}\eta^{kl}\big) - 4\eta^{mn}\big(\cancelto{(1)}{\eta^{ij}\eta^{kl}} - \cancelto{(2)}{\eta^{ik}\eta^{jl}} + \cancelto{(3)}{\eta^{il}\eta^{jk}}\big) \\
&\qquad - 4\eta^{jk}\big(\cancelto{(6)}{\eta^{il}\eta^{mn}} - \cancelto{(4)}{\eta^{im}\eta^{ln}} + \cancelto{(5)}{\eta^{in}\eta^{lm}}\big) + \cancelto{(6)}{4\eta^{jk}\eta^{mn}\eta^{il}}\Big\} \\
&\quad = 16\Big\{\eta^{ij}\big(-\eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big) - \eta^{ik}\big(-\eta^{jm}\eta^{ln} + \eta^{jn}\eta^{lm}\big) + \eta^{il}\big(-\eta^{jm}\eta^{kn} + \eta^{jn}\eta^{km}\big) \\
&\qquad - \eta^{im}\big(-\eta^{jl}\eta^{kn} + \eta^{jn}\eta^{kl}\big) + \eta^{in}\big(-\eta^{jl}\eta^{km} + \eta^{jm}\eta^{kl}\big)\Big\}
\end{aligned}
$$

Finally, for the fourth identity we again make repeated use of the relation $[\gamma^i,\gamma^j] = 2(\gamma^i\gamma^j - \eta^{ij}\mathrm{id}_{\mathbb{C}^4})$ resulting from $\gamma^i\gamma^j = \frac{1}{2}[\gamma^i,\gamma^j] + \frac{1}{2}\{\gamma^i,\gamma^j\} = \frac{1}{2}[\gamma^i,\gamma^j] + \eta^{ij}\mathrm{id}_{\mathbb{C}^4}$. In this way we find

$$
\begin{aligned}
&\mathrm{Tr}\left[[\gamma^i,\gamma^j][\gamma^k,\gamma^l][\gamma^m,\gamma^n]\right] = \\
&\quad = 8\,\mathrm{Tr}\left[(\gamma^i\gamma^j - \eta^{ij}\mathrm{id}_{\mathbb{C}^4})(\gamma^k\gamma^l - \eta^{kl}\mathrm{id}_{\mathbb{C}^4})(\gamma^m\gamma^n - \eta^{mn}\mathrm{id}_{\mathbb{C}^4})\right] \\
&\quad = 8\Big\{\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\right] - \eta^{mn}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\right] - \eta^{kl}\Big(\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^m\gamma^n\right] - \eta^{mn}\,\mathrm{Tr}\left[\gamma^i\gamma^j\right]\Big) \\
&\qquad - \eta^{ij}\Big(\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\right] - \eta^{mn}\,\mathrm{Tr}\left[\gamma^k\gamma^l\right] - \eta^{kl}\,\mathrm{Tr}\left[\gamma^m\gamma^n\right] + \eta^{kl}\eta^{mn}\,\mathrm{Tr}\left[\mathrm{id}_{\mathbb{C}^4}\right]\Big)\Big\} \\
&\quad \overset{\text{(B.3a)}}{\underset{\text{(B.7a)}}{=}} 8\Big\{4\eta^{ij}\big(\eta^{kl}\eta^{mn} - \eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big) - 4\eta^{ik}\big(\eta^{jl}\eta^{mn} - \eta^{jm}\eta^{ln} + \eta^{jn}\eta^{lm}\big) \\
&\qquad + 4\eta^{il}\big(\eta^{jk}\eta^{mn} - \eta^{jm}\eta^{kn} + \eta^{jn}\eta^{km}\big) - 4\eta^{im}\big(\eta^{jk}\eta^{ln} - \eta^{jl}\eta^{kn} + \eta^{jn}\eta^{kl}\big) \\
&\qquad + 4\eta^{in}\big(\eta^{jk}\eta^{lm} - \eta^{jl}\eta^{km} + \eta^{jm}\eta^{kl}\big) - 4\eta^{mn}\big(\eta^{ij}\eta^{kl} - \eta^{ik}\eta^{jl} + \eta^{il}\eta^{jk}\big) \\
&\qquad - \eta^{kl}\Big(4\big(\eta^{ij}\eta^{mn} - \eta^{im}\eta^{jn} + \eta^{in}\eta^{jm}\big) - 4\eta^{mn}\eta^{ij}\Big) \\
&\qquad - \eta^{ij}\Big(4\big(\eta^{kl}\eta^{mn} - \eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big) - 4\eta^{mn}\eta^{kl} - 4\eta^{kl}\eta^{mn} + 4\eta^{kl}\eta^{mn}\Big)\Big\} \\
&\quad = 8\Big\{4\eta^{ij}\big(\eta^{kl}\eta^{mn} - \cancelto{(1)}{\eta^{km}\eta^{ln}} + \eta^{kn}\eta^{lm}\big) - 4\eta^{ik}\big(\cancelto{(2)}{\eta^{jl}\eta^{mn}} - \eta^{jm}\eta^{ln} + \eta^{jn}\eta^{lm}\big) \\
&\qquad + 4\eta^{il}\big(\cancelto{(3)}{\eta^{jk}\eta^{mn}} - \eta^{jm}\eta^{kn} + \eta^{jn}\eta^{km}\big) - 4\eta^{im}\big(\eta^{jk}\eta^{ln} - \eta^{jl}\eta^{kn} + \cancelto{(4)}{\eta^{jn}\eta^{kl}}\big) \\
&\qquad + 4\eta^{in}\big(\eta^{jk}\eta^{lm} - \eta^{jl}\eta^{km} + \cancelto{(5)}{\eta^{jm}\eta^{kl}}\big) - 4\eta^{mn}\big(\cancelto{(6)}{\eta^{ij}\eta^{kl}} - \cancelto{(2)}{\eta^{ik}\eta^{jl}} + \cancelto{(3)}{\eta^{il}\eta^{jk}}\big) \\
&\qquad - \eta^{kl}\Big(4\big(\cancelto{(7)}{\eta^{ij}\eta^{mn}} - \cancelto{(4)}{\eta^{im}\eta^{jn}} + \cancelto{(5)}{\eta^{in}\eta^{jm}}\big) - \cancelto{(7)}{4\eta^{mn}\eta^{ij}}\Big) \\
&\qquad - \eta^{ij}\Big(4\big(\eta^{kl}\eta^{mn} - \cancelto{(1)}{\eta^{km}\eta^{ln}} + \eta^{kn}\eta^{lm}\big) - \cancelto{(6)}{4\eta^{mn}\eta^{kl}} - \cancelto{(8)}{4\eta^{kl}\eta^{mn}} + \cancelto{(8)}{4\eta^{kl}\eta^{mn}}\Big)\Big\}
\end{aligned}
$$

$$= 8\Big\{ -4\eta^{ik}\big(-\eta^{jm}\eta^{ln}+\eta^{jn}\eta^{lm}\big)+4\eta^{il}\big(-\eta^{jm}\eta^{kn}+\eta^{jn}\eta^{km}\big) - 4\eta^{im}\big(\eta^{jk}\eta^{ln}-\eta^{jl}\eta^{kn}\big)+4\eta^{in}\big(\eta^{jk}\eta^{lm}-\eta^{jl}\eta^{km}\big)\Big\}$$

This concludes the proof. □

B.1.4 Trace Identities involving eight Dirac Matrices

In the case where there are eight Dirac matrices, there are again several possible combinations.

Proposition B.1.4 (Trace Identities involving eight Dirac Matrices)

For eight Dirac matrices we have the following two identities which are relevant for the evaluation of the second term in (3.23b)

$$\begin{aligned}\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] &= \\ &= \eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right]-\eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right]+\eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^m\gamma^n\gamma^p\gamma^q\right] \\ &\quad -\eta^{im}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^n\gamma^p\gamma^q\right]+\eta^{in}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^p\gamma^q\right]-\eta^{ip}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^q\right] \\ &\quad +\eta^{iq}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\right] \end{aligned} \tag{B.9a}$$

$$\begin{aligned}\mathrm{Tr}\left[[\gamma^i,\gamma^j][\gamma^k,\gamma^l][\gamma^m,\gamma^n][\gamma^p,\gamma^q]\right] &= \\ = 64\Big\{ &-\eta^{ik}\Big\{\eta^{jl}\big(-\eta^{mp}\eta^{nq}+\eta^{mq}\eta^{np}\big)-\eta^{jm}\big(-\eta^{lp}\eta^{nq}+\eta^{lq}\eta^{np}\big) \\ &\quad +\eta^{jn}\big(-\eta^{lp}\eta^{mq}+\eta^{lq}\eta^{mp}\big)-\eta^{jp}\big(\eta^{lm}\eta^{nq}-\eta^{ln}\eta^{mq}\big) \\ &\quad +\eta^{jq}\big(\eta^{lm}\eta^{np}-\eta^{ln}\eta^{mp}\big)\Big\} \\ &+\eta^{il}\Big\{\eta^{jk}\big(-\eta^{mp}\eta^{nq}+\eta^{mq}\eta^{np}\big)-\eta^{jm}\big(-\eta^{kp}\eta^{nq}+\eta^{kq}\eta^{np}\big) \\ &\quad +\eta^{jn}\big(-\eta^{kp}\eta^{mq}+\eta^{kq}\eta^{mp}\big)-\eta^{jp}\big(\eta^{km}\eta^{nq}-\eta^{kn}\eta^{mq}\big) \\ &\quad +\eta^{jq}\big(\eta^{km}\eta^{np}-\eta^{kn}\eta^{mp}\big)\Big\} \\ &-\eta^{im}\Big\{\eta^{jk}\big(-\eta^{lp}\eta^{nq}+\eta^{lq}\eta^{np}\big)-\eta^{jl}\big(-\eta^{kp}\eta^{nq}+\eta^{kq}\eta^{np}\big) \\ &\quad +\eta^{jn}\big(-\eta^{kp}\eta^{lq}+\eta^{kq}\eta^{lp}\big)-\eta^{jp}\big(-\eta^{kn}\eta^{lq}+\eta^{kq}\eta^{ln}\big) \\ &\quad +\eta^{jq}\big(-\eta^{kn}\eta^{lp}+\eta^{kp}\eta^{ln}\big)\Big\} \\ &+\eta^{in}\Big\{\eta^{jk}\big(-\eta^{lp}\eta^{mq}+\eta^{lq}\eta^{mp}\big)-\eta^{jl}\big(-\eta^{kp}\eta^{mq}+\eta^{kq}\eta^{mp}\big) \\ &\quad +\eta^{jm}\big(-\eta^{kp}\eta^{lq}+\eta^{kq}\eta^{lp}\big)-\eta^{jp}\big(-\eta^{km}\eta^{lq}+\eta^{kq}\eta^{lm}\big) \\ &\quad +\eta^{jq}\big(-\eta^{km}\eta^{lp}+\eta^{kp}\eta^{lm}\big)\Big\} \\ &-\eta^{ip}\Big\{\eta^{jk}\big(\eta^{lm}\eta^{nq}-\eta^{ln}\eta^{mq}\big)-\eta^{jl}\big(\eta^{km}\eta^{nq}-\eta^{kn}\eta^{mq}\big) \\ &\quad +\eta^{jm}\big(-\eta^{kn}\eta^{lq}+\eta^{kq}\eta^{ln}\big)-\eta^{jn}\big(-\eta^{km}\eta^{lq}+\eta^{kq}\eta^{lm}\big) \\ &\quad +\eta^{jq}\big(-\eta^{km}\eta^{ln}+\eta^{kn}\eta^{lm}\big)\Big\} \\ &+\eta^{iq}\Big\{\eta^{jk}\big(\eta^{lm}\eta^{np}-\eta^{ln}\eta^{mp}\big)-\eta^{jl}\big(\eta^{km}\eta^{np}-\eta^{kn}\eta^{mp}\big) \\ &\quad +\eta^{jm}\big(-\eta^{kn}\eta^{lp}+\eta^{kp}\eta^{ln}\big)-\eta^{jn}\big(-\eta^{km}\eta^{lp}+\eta^{kp}\eta^{lm}\big) \\ &\quad +\eta^{jp}\big(-\eta^{km}\eta^{ln}+\eta^{kn}\eta^{lm}\big)\Big\}\Big\} \end{aligned} \tag{B.9b}$$

Proof. To prove the first identity, we make repeated use of the relation $\gamma^i\gamma^j = 2\eta^{ij}\mathrm{id}_{\mathbb{C}^4} - \gamma^j\gamma^i$ resulting from $\{\gamma^i,\gamma^j\} = 2\eta^{ij}\mathrm{id}_{\mathbb{C}^4}$. In this way we find

$$\begin{aligned}
&\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] = \\
&\quad = \mathrm{Tr}\left[(2\eta^{ij} - \gamma^j\gamma^i)\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] \\
&\quad = 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] - \mathrm{Tr}\left[\gamma^j(2\eta^{ik} - \gamma^k\gamma^i)\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] \\
&\quad = 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] - 2\eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] + \mathrm{Tr}\left[\gamma^j\gamma^k(2\eta^{il} - \gamma^l\gamma^i)\gamma^m\gamma^n\gamma^p\gamma^q\right] \\
&\quad = 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] - 2\eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] + 2\eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^m\gamma^n\gamma^p\gamma^q\right] \\
&\qquad\qquad - \mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l(2\eta^{im} - \gamma^m\gamma^i)\gamma^n\gamma^p\gamma^q\right] \\
&\quad = 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] - 2\eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] + 2\eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^m\gamma^n\gamma^p\gamma^q\right] \\
&\qquad - 2\eta^{im}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^n\gamma^p\gamma^q\right] + \mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m(2\eta^{in} - \gamma^n\gamma^i)\gamma^p\gamma^q\right] \\
&\quad = 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] - 2\eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] + 2\eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^m\gamma^n\gamma^p\gamma^q\right] \\
&\qquad - 2\eta^{im}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^n\gamma^p\gamma^q\right] + 2\eta^{in}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^p\gamma^q\right] - \mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n(2\eta^{ip} - \gamma^p\gamma^i)\gamma^q\right] \\
&\quad = 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] - 2\eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] + 2\eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^m\gamma^n\gamma^p\gamma^q\right] \\
&\qquad - 2\eta^{im}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^n\gamma^p\gamma^q\right] + 2\eta^{in}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^p\gamma^q\right] - 2\eta^{ip}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^q\right] \\
&\qquad\qquad + \mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p(2\eta^{iq} - \gamma^q\gamma^i)\right] \\
&\quad = 2\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] - 2\eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] + 2\eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^m\gamma^n\gamma^p\gamma^q\right] \\
&\qquad - 2\eta^{im}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^n\gamma^p\gamma^q\right] + 2\eta^{in}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^p\gamma^q\right] - 2\eta^{ip}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^q\right] \\
&\qquad\qquad + 2\eta^{iq}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\right] - \mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\gamma^i\right]
\end{aligned}$$

By exploiting the cyclicity of the trace, the last term can be combined with the left-hand side which thus, together with (B.7a), yields

$$\begin{aligned}
&\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] = \\
&\quad \overset{\text{(B.7a)}}{=} \eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] - \eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] + \eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^m\gamma^n\gamma^p\gamma^q\right] \\
&\qquad - \eta^{im}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^n\gamma^p\gamma^q\right] + \eta^{in}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^p\gamma^q\right] - \eta^{ip}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^q\right] \\
&\qquad\qquad + \eta^{iq}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\right] \qquad \text{(B.10)}
\end{aligned}$$

For the second identity we again make repeated use of the relation $[\gamma^i,\gamma^j] = 2(\gamma^i\gamma^j - \eta^{ij}\mathrm{id}_{\mathbb{C}^4})$ resulting from $\gamma^i\gamma^j = \frac{1}{2}[\gamma^i,\gamma^j] + \frac{1}{2}\{\gamma^i,\gamma^j\} = \frac{1}{2}[\gamma^i,\gamma^j] + \eta^{ij}\mathrm{id}_{\mathbb{C}^4}$. In this way we find

$$\begin{aligned}
&\mathrm{Tr}\left[[\gamma^i,\gamma^j][\gamma^k,\gamma^l][\gamma^m,\gamma^n][\gamma^p,\gamma^q]\right] = \\
&\quad = 16\,\mathrm{Tr}\left[(\gamma^i\gamma^j - \eta^{ij})(\gamma^k\gamma^l - \eta^{kl})(\gamma^m\gamma^n - \eta^{mn})(\gamma^p\gamma^q - \eta^{pq})\right] \\
&\quad = 16\,\mathrm{Tr}\left[(\gamma^i\gamma^j\gamma^k\gamma^l - \eta^{kl}\gamma^i\gamma^j - \eta^{ij}\gamma^k\gamma^l + \eta^{ij}\eta^{kl})(\gamma^m\gamma^n\gamma^p\gamma^q - \eta^{pq}\gamma^m\gamma^n \right. \\
&\qquad\qquad \left. - \eta^{mn}\gamma^p\gamma^q + \eta^{mn}\eta^{pq})\right] \\
&\quad = 16\Big\{\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] - \eta^{pq}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\right] \\
&\qquad - \eta^{mn}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^p\gamma^q\right] + \eta^{mn}\eta^{pq}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\right] \\
&\qquad - \eta^{kl}\Big(\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^m\gamma^n\gamma^p\gamma^q\right] - \eta^{pq}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^m\gamma^n\right] - \eta^{mn}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^p\gamma^q\right] \\
&\qquad\qquad + \eta^{mn}\eta^{pq}\,\mathrm{Tr}\left[\gamma^i\gamma^j\right]\Big) \\
&\qquad - \eta^{ij}\Big(\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] - \eta^{pq}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\right] - \eta^{mn}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^p\gamma^q\right]
\end{aligned}$$

$$
\begin{aligned}
&\qquad\qquad + \eta^{mn}\eta^{pq}\,\mathrm{Tr}\left[\gamma^k\gamma^l\right]\Big) \\
&\quad + \eta^{ij}\eta^{kl}\Big(\mathrm{Tr}\left[\gamma^m\gamma^n\gamma^p\gamma^q\right] - \eta^{pq}\,\mathrm{Tr}\left[\gamma^m\gamma^n\right] - \eta^{mn}\,\mathrm{Tr}\left[\gamma^p\gamma^q\right] + \eta^{mn}\eta^{pq}\,\mathrm{Tr}\left[\mathrm{id}_{\mathbb{C}^4}\right]\Big)\Big\}
\end{aligned}
$$

$$
\begin{aligned}
= 16\Big\{ & \cancelto{(1)}{\eta^{ij}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right]} - \eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] + \eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^m\gamma^n\gamma^p\gamma^q\right] \\
& - \eta^{im}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^n\gamma^p\gamma^q\right] + \eta^{in}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^p\gamma^q\right] - \eta^{ip}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^q\right] \\
& + \eta^{iq}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\right] - \eta^{pq}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\right] \\
& - \eta^{mn}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^p\gamma^q\right] + \eta^{mn}\eta^{pq}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\right] \\
& - \eta^{kl}\Big(\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^m\gamma^n\gamma^p\gamma^q\right] - \eta^{pq}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^m\gamma^n\right] - \eta^{mn}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^p\gamma^q\right] \\
& \qquad\qquad + \eta^{mn}\eta^{pq}\,\mathrm{Tr}\left[\gamma^i\gamma^j\right]\Big) \\
& - \eta^{ij}\Big(\cancelto{(1)}{\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right]} - \eta^{pq}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\right] - \eta^{mn}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^p\gamma^q\right] \\
& \qquad\qquad + \eta^{mn}\eta^{pq}\,\mathrm{Tr}\left[\gamma^k\gamma^l\right]\Big) \\
& + \eta^{ij}\eta^{kl}\Big(\mathrm{Tr}\left[\gamma^m\gamma^n\gamma^p\gamma^q\right] - \eta^{pq}\,\mathrm{Tr}\left[\gamma^m\gamma^n\right] - \cancelto{(2)}{\eta^{mn}\,\mathrm{Tr}\left[\gamma^p\gamma^q\right]} + \cancelto{(2)}{\eta^{mn}\eta^{pq}\,\mathrm{Tr}\left[\mathrm{id}_{\mathbb{C}^4}\right]}\Big)\Big\}
\end{aligned}
$$

$$
\begin{aligned}
16\Big\{ & - \eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] + \eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^m\gamma^n\gamma^p\gamma^q\right] - \eta^{im}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^n\gamma^p\gamma^q\right] \\
& + \eta^{in}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^p\gamma^q\right] - \eta^{ip}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^q\right] + \eta^{iq}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\right] \\
& - \eta^{pq}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\right] - \eta^{mn}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^p\gamma^q\right] - \eta^{kl}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^m\gamma^n\gamma^p\gamma^q\right] \\
& + \eta^{mn}\eta^{pq}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\right] + \eta^{kl}\eta^{pq}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^m\gamma^n\right] + \eta^{kl}\eta^{mn}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^p\gamma^q\right] \\
& + \eta^{ij}\eta^{pq}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^m\gamma^n\right] + \eta^{ij}\eta^{mn}\,\mathrm{Tr}\left[\gamma^k\gamma^l\gamma^p\gamma^q\right] + \eta^{ij}\eta^{kl}\,\mathrm{Tr}\left[\gamma^m\gamma^n\gamma^p\gamma^q\right] \\
& - \eta^{kl}\eta^{mn}\eta^{pq}\,\mathrm{Tr}\left[\gamma^i\gamma^j\right] - \eta^{ij}\eta^{mn}\eta^{pq}\,\mathrm{Tr}\left[\gamma^k\gamma^l\right] - \eta^{ij}\eta^{kl}\eta^{pq}\,\mathrm{Tr}\left[\gamma^m\gamma^n\right]\Big\}
\end{aligned}
$$

$$
\begin{aligned}
\overset{(B.1a)}{\underset{(B.3a)}{=}} 16\Big\{ & - \eta^{ik}\,\mathrm{Tr}\left[\gamma^j\gamma^l\gamma^m\gamma^n\gamma^p\gamma^q\right] + \eta^{il}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^m\gamma^n\gamma^p\gamma^q\right] - \eta^{im}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^n\gamma^p\gamma^q\right] \\
& + \eta^{in}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^p\gamma^q\right] - \eta^{ip}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^q\right] + \eta^{iq}\,\mathrm{Tr}\left[\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\gamma^p\right] \\
& - \eta^{pq}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^m\gamma^n\right] - \eta^{mn}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^k\gamma^l\gamma^p\gamma^q\right] - \eta^{kl}\,\mathrm{Tr}\left[\gamma^i\gamma^j\gamma^m\gamma^n\gamma^p\gamma^q\right] \\
& + 4\eta^{mn}\eta^{pq}\left(\cancelto{(1)}{\eta^{ij}\eta^{kl}} - \eta^{ik}\eta^{jl} + \eta^{il}\eta^{jk}\right) + 4\eta^{kl}\eta^{pq}\left(\eta^{ij}\eta^{mn} - \eta^{im}\eta^{jn} + \eta^{in}\eta^{jm}\right) \\
& + 4\eta^{kl}\eta^{mn}\left(\cancelto{(2)}{\eta^{ij}\eta^{pq}} - \eta^{ip}\eta^{jq} + \eta^{iq}\eta^{jp}\right) + 4\eta^{ij}\eta^{pq}\left(\eta^{kl}\eta^{mn} - \eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\right) \\
& + 4\eta^{ij}\eta^{mn}\left(\cancelto{(3)}{\eta^{kl}\eta^{pq}} - \eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\right) + 4\eta^{ij}\eta^{kl}\left(\eta^{mn}\eta^{pq} - \eta^{mp}\eta^{nq} + \eta^{mq}\eta^{np}\right) \\
& \qquad - \cancelto{(1)}{4\eta^{kl}\eta^{mn}\eta^{pq}\eta^{ij}} - \cancelto{(2)}{4\eta^{ij}\eta^{mn}\eta^{pq}\eta^{kl}} - \cancelto{(3)}{4\eta^{ij}\eta^{kl}\eta^{pq}\eta^{mn}}\Big\}
\end{aligned}
$$

$$
\begin{aligned}
\overset{(B.7a)}{=} 16\Big\{ & - \eta^{ik}\Big\{4\eta^{jl}\left(\cancelto{(1)}{\eta^{mn}\eta^{pq}} - \eta^{mp}\eta^{nq} + \eta^{mq}\eta^{np}\right) - 4\eta^{jm}\left(\cancelto{(2)}{\eta^{ln}\eta^{pq}} - \eta^{lp}\eta^{nq} + \eta^{lq}\eta^{np}\right) \\
& \quad + 4\eta^{jn}\left(\cancelto{(3)}{\eta^{lm}\eta^{pq}} - \eta^{lp}\eta^{mq} + \eta^{lq}\eta^{mp}\right) - 4\eta^{jp}\left(\eta^{lm}\eta^{nq} - \eta^{ln}\eta^{mq} + \cancelto{(4)}{\eta^{lq}\eta^{mn}}\right) \\
& \qquad + 4\eta^{jq}\left(\eta^{lm}\eta^{np} - \eta^{ln}\eta^{mp} + \cancelto{(5)}{\eta^{lp}\eta^{mn}}\right)\Big\} \\
& + \eta^{il}\Big\{4\eta^{jk}\left(\cancelto{(6)}{\eta^{mn}\eta^{pq}} - \eta^{mp}\eta^{nq} + \eta^{mq}\eta^{np}\right) - 4\eta^{jm}\left(\cancelto{(7)}{\eta^{kn}\eta^{pq}} - \eta^{kp}\eta^{nq} + \eta^{kq}\eta^{np}\right) \\
& \quad + 4\eta^{jn}\left(\cancelto{(8)}{\eta^{km}\eta^{pq}} - \eta^{kp}\eta^{mq} + \eta^{kq}\eta^{mp}\right) - 4\eta^{jp}\left(\eta^{km}\eta^{nq} - \eta^{kn}\eta^{mq} + \cancelto{(9)}{\eta^{kq}\eta^{mn}}\right) \\
& \qquad + 4\eta^{jq}\left(\eta^{km}\eta^{np} - \eta^{kn}\eta^{mp} + \cancelto{(10)}{\eta^{kp}\eta^{mn}}\right)\Big\}
\end{aligned}
$$

$$
\begin{aligned}
&- \eta^{im}\Big\{4\eta^{jk}\big(\cancelto{(11)}{\eta^{ln}\eta^{pq}} - \eta^{lp}\eta^{nq} + \eta^{lq}\eta^{np}\big) - 4\eta^{jl}\big(\cancelto{(12)}{\eta^{kn}\eta^{pq}} - \eta^{kp}\eta^{nq} + \eta^{kq}\eta^{np}\big) \\
&\qquad + 4\eta^{jn}\big(\cancelto{(13)}{\eta^{kl}\eta^{pq}} - \eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big) - 4\eta^{jp}\big(\cancelto{(14)}{\eta^{kl}\eta^{nq}} - \eta^{kn}\eta^{lq} + \eta^{kq}\eta^{ln}\big) \\
&\qquad\qquad + 4\eta^{jq}\big(\cancelto{(15)}{\eta^{kl}\eta^{np}} - \eta^{kn}\eta^{lp} + \eta^{kp}\eta^{ln}\big)\Big\} \\
&+ \eta^{in}\Big\{4\eta^{jk}\big(\cancelto{(16)}{\eta^{lm}\eta^{pq}} - \eta^{lp}\eta^{mq} + \eta^{lq}\eta^{mp}\big) - 4\eta^{jl}\big(\cancelto{(17)}{\eta^{km}\eta^{pq}} - \eta^{kp}\eta^{mq} + \eta^{kq}\eta^{mp}\big) \\
&\qquad + 4\eta^{jm}\big(\cancelto{(18)}{\eta^{kl}\eta^{pq}} - \eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big) - 4\eta^{jp}\big(\cancelto{(19)}{\eta^{kl}\eta^{mq}} - \eta^{km}\eta^{lq} + \eta^{kq}\eta^{lm}\big) \\
&\qquad\qquad + 4\eta^{jq}\big(\cancelto{(20)}{\eta^{kl}\eta^{mp}} - \eta^{km}\eta^{lp} + \eta^{kp}\eta^{lm}\big)\Big\} \\
&- \eta^{ip}\Big\{4\eta^{jk}\big(\eta^{lm}\eta^{nq} - \eta^{ln}\eta^{mq} + \cancelto{(21)}{\eta^{lq}\eta^{mn}}\big) - 4\eta^{jl}\big(\eta^{km}\eta^{nq} - \eta^{kn}\eta^{mq} + \cancelto{(22)}{\eta^{kq}\eta^{mn}}\big) \\
&\qquad + 4\eta^{jm}\big(\cancelto{(23)}{\eta^{kl}\eta^{nq}} - \eta^{kn}\eta^{lq} + \eta^{kq}\eta^{ln}\big) - 4\eta^{jn}\big(\cancelto{(24)}{\eta^{kl}\eta^{mq}} - \eta^{km}\eta^{lq} + \eta^{kq}\eta^{lm}\big) \\
&\qquad\qquad + 4\eta^{jq}\big(\cancelto{(25)}{\eta^{kl}\eta^{mn}} - \eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big)\Big\} \\
&+ \eta^{iq}\Big\{4\eta^{jk}\big(\eta^{lm}\eta^{np} - \eta^{ln}\eta^{mp} + \cancelto{(26)}{\eta^{lp}\eta^{mn}}\big) - 4\eta^{jl}\big(\eta^{km}\eta^{np} - \eta^{kn}\eta^{mp} + \cancelto{(27)}{\eta^{kp}\eta^{mn}}\big) \\
&\qquad + 4\eta^{jm}\big(\cancelto{(28)}{\eta^{kl}\eta^{np}} - \eta^{kn}\eta^{lp} + \eta^{kp}\eta^{ln}\big) - 4\eta^{jn}\big(\cancelto{(29)}{\eta^{kl}\eta^{mp}} - \eta^{km}\eta^{lp} + \eta^{kp}\eta^{lm}\big) \\
&\qquad\qquad + 4\eta^{jp}\big(\cancelto{(30)}{\eta^{kl}\eta^{mn}} - \eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big)\Big\} \\
&- \eta^{pq}\Big\{\cancelto{(31)}{4\eta^{ij}\big(\eta^{kl}\eta^{mn} - \eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big)} - 4\eta^{ik}\big(\cancelto{(1)}{\eta^{jl}\eta^{mn}} - \cancelto{(2)}{\eta^{jm}\eta^{ln}} + \cancelto{(3)}{\eta^{jn}\eta^{lm}}\big) \\
&\qquad + 4\eta^{il}\big(\cancelto{(6)}{\eta^{jk}\eta^{mn}} - \cancelto{(7)}{\eta^{jm}\eta^{kn}} + \cancelto{(8)}{\eta^{jn}\eta^{km}}\big) - 4\eta^{im}\big(\cancelto{(11)}{\eta^{jk}\eta^{ln}} - \cancelto{(12)}{\eta^{jl}\eta^{kn}} + \cancelto{(13)}{\eta^{jn}\eta^{kl}}\big) \\
&\qquad\qquad + 4\eta^{in}\big(\cancelto{(16)}{\eta^{jk}\eta^{lm}} - \cancelto{(17)}{\eta^{jl}\eta^{km}} + \cancelto{(18)}{\eta^{jm}\eta^{kl}}\big)\Big\} \\
&- \eta^{mn}\Big\{4\eta^{ij}\big(\cancelto{(33)}{\eta^{kl}\eta^{pq}} \cancelto{(32)}{- \eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}}\big) - 4\eta^{ik}\big(\cancelto{(4)}{\eta^{jl}\eta^{pq}} - \cancelto{(4)}{\eta^{jp}\eta^{lq}} + \cancelto{(5)}{\eta^{jq}\eta^{lp}}\big) \\
&\qquad + 4\eta^{il}\big(\cancelto{(35)}{\eta^{jk}\eta^{pq}} - \cancelto{(9)}{\eta^{jp}\eta^{kq}} + \cancelto{(10)}{\eta^{jq}\eta^{kp}}\big) - 4\eta^{ip}\big(\cancelto{(21)}{\eta^{jk}\eta^{lq}} - \cancelto{(22)}{\eta^{jl}\eta^{kq}} + \cancelto{(36)}{\eta^{jq}\eta^{kl}}\big) \\
&\qquad\qquad + 4\eta^{iq}\big(\cancelto{(6)}{\eta^{jk}\eta^{lp}} - \cancelto{(27)}{\eta^{jl}\eta^{kp}} + \cancelto{(37)}{\eta^{jp}\eta^{kl}}\big)\Big\} \\
&- \eta^{kl}\Big\{\cancelto{(38)}{4\eta^{ij}\big(\eta^{mn}\eta^{pq} - \eta^{mp}\eta^{nq} + \eta^{mq}\eta^{np}\big)} - 4\eta^{im}\big(\cancelto{(39)}{\eta^{jn}\eta^{pq}} - \cancelto{(14)}{\eta^{jp}\eta^{nq}} + \cancelto{(15)}{\eta^{jq}\eta^{np}}\big) \\
&\qquad + 4\eta^{in}\big(\cancelto{(40)}{\eta^{jm}\eta^{pq}} - \cancelto{(19)}{\eta^{jp}\eta^{mq}} + \cancelto{(20)}{\eta^{jq}\eta^{mp}}\big) - 4\eta^{ip}\big(\cancelto{(23)}{\eta^{jm}\eta^{nq}} - \cancelto{(24)}{\eta^{jn}\eta^{mq}} + \cancelto{(25)}{\eta^{jq}\eta^{mn}}\big) \\
&\qquad\qquad + 4\eta^{iq}\big(\cancelto{(28)}{\eta^{jm}\eta^{np}} - \cancelto{(29)}{\eta^{jn}\eta^{mp}} + \cancelto{(30)}{\eta^{jp}\eta^{mn}}\big)\Big\} \\
&+ 4\eta^{mn}\eta^{pq}\big(-\cancelto{(34)}{\eta^{ik}\eta^{jl}} + \cancelto{(35)}{\eta^{il}\eta^{jk}}\big) + 4\eta^{kl}\eta^{pq}\big(\cancelto{(33)}{\eta^{ij}\eta^{mn}} - \cancelto{(39)}{\eta^{im}\eta^{jn}} + \cancelto{(40)}{\eta^{in}\eta^{jm}}\big) \\
&\qquad + 4\eta^{kl}\eta^{mn}\big(-\cancelto{(36)}{\eta^{ip}\eta^{jq}} + \cancelto{(37)}{\eta^{iq}\eta^{jp}}\big) + \cancelto{(31)}{4\eta^{ij}\eta^{pq}\big(\eta^{kl}\eta^{mn} - \eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big)} \\
&\qquad\quad + \cancelto{(32)}{4\eta^{ij}\eta^{mn}\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big)} + \cancelto{(38)}{4\eta^{ij}\eta^{kl}\big(\eta^{mn}\eta^{pq} - \eta^{mp}\eta^{nq} + \eta^{mq}\eta^{np}\big)}\Big\} \\
= 64\Big\{ &- \eta^{ik}\Big\{\eta^{jl}\big(-\eta^{mp}\eta^{nq} + \eta^{mq}\eta^{np}\big) - \eta^{jm}\big(-\eta^{lp}\eta^{nq} + \eta^{lq}\eta^{np}\big) \\
&\qquad + \eta^{jn}\big(-\eta^{lp}\eta^{mq} + \eta^{lq}\eta^{mp}\big) - \eta^{jp}\big(\eta^{lm}\eta^{nq} - \eta^{ln}\eta^{mq}\big)
\end{aligned}
$$

$$
\begin{aligned}
&\qquad\qquad\qquad\qquad\qquad + \eta^{jq}\big(\eta^{lm}\eta^{np} - \eta^{ln}\eta^{mp}\big)\Big\} \\
&+ \eta^{il}\Big\{\eta^{jk}\big(-\eta^{mp}\eta^{nq} + \eta^{mq}\eta^{np}\big) - \eta^{jm}\big(-\eta^{kp}\eta^{nq} + \eta^{kq}\eta^{np}\big) \\
&\qquad + \eta^{jn}\big(-\eta^{kp}\eta^{mq} + \eta^{kq}\eta^{mp}\big) - \eta^{jp}\big(\eta^{km}\eta^{nq} - \eta^{kn}\eta^{mq}\big) \\
&\qquad\qquad\qquad\qquad\qquad + \eta^{jq}\big(\eta^{km}\eta^{np} - \eta^{kn}\eta^{mp}\big)\Big\} \\
&- \eta^{im}\Big\{\eta^{jk}\big(-\eta^{lp}\eta^{nq} + \eta^{lq}\eta^{np}\big) - \eta^{jl}\big(-\eta^{kp}\eta^{nq} + \eta^{kq}\eta^{np}\big) \\
&\qquad + \eta^{jn}\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big) - \eta^{jp}\big(-\eta^{kn}\eta^{lq} + \eta^{kq}\eta^{ln}\big) \\
&\qquad\qquad\qquad\qquad\qquad + \eta^{jq}\big(-\eta^{kn}\eta^{lp} + \eta^{kp}\eta^{ln}\big)\Big\} \\
&+ \eta^{in}\Big\{\eta^{jk}\big(-\eta^{lp}\eta^{mq} + \eta^{lq}\eta^{mp}\big) - \eta^{jl}\big(-\eta^{kp}\eta^{mq} + \eta^{kq}\eta^{mp}\big) \\
&\qquad + \eta^{jm}\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big) - \eta^{jp}\big(-\eta^{km}\eta^{lq} + \eta^{kq}\eta^{lm}\big) \\
&\qquad\qquad\qquad\qquad\qquad + \eta^{jq}\big(-\eta^{km}\eta^{lp} + \eta^{kp}\eta^{lm}\big)\Big\} \\
&- \eta^{ip}\Big\{\eta^{jk}\big(\eta^{lm}\eta^{nq} - \eta^{ln}\eta^{mq}\big) - \eta^{jl}\big(\eta^{km}\eta^{nq} - \eta^{kn}\eta^{mq}\big) \\
&\qquad + \eta^{jm}\big(-\eta^{kn}\eta^{lq} + \eta^{kq}\eta^{ln}\big) - \eta^{jn}\big(-\eta^{km}\eta^{lq} + \eta^{kq}\eta^{lm}\big) \\
&\qquad\qquad\qquad\qquad\qquad + \eta^{jq}\big(-\eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big)\Big\} \\
&+ \eta^{iq}\Big\{\eta^{jk}\big(\eta^{lm}\eta^{np} - \eta^{ln}\eta^{mp}\big) - \eta^{jl}\big(\eta^{km}\eta^{np} - \eta^{kn}\eta^{mp}\big) \\
&\qquad + \eta^{jm}\big(-\eta^{kn}\eta^{lp} + \eta^{kp}\eta^{ln}\big) - \eta^{jn}\big(-\eta^{km}\eta^{lp} + \eta^{kp}\eta^{lm}\big) \\
&\qquad\qquad\qquad\qquad\qquad + \eta^{jp}\big(-\eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big)\Big\}\Big\}
\end{aligned}
$$

This concludes the proof. □

B.2 Derivation of (3.22b) in Lemma 3.3.7

Having derived all the trace identities for commutators of Dirac matrices which are necessary to evaluate the second term in (3.23b), we are now ready to complete the proof of (3.22b) in Lemma 3.3.7.

Continuation of Lemma 3.3.7 (Derivation of (3.22b))

The second variation of the eigenvalues of the regularized closed chain evaluates to

$$
\begin{aligned}
&\delta^2\lambda^\varepsilon_\pm(x,y) = \\
&= \mathrm{Re}\Big[2\big(\overline{v^i_\varepsilon}\,\delta^2 v^\varepsilon_i\big) + 2\overline{s^\varepsilon}\,\delta^2 s^\varepsilon + \big(\delta v^i_\varepsilon\,\overline{\delta v^\varepsilon_i}\big) + \delta s^\varepsilon\,\overline{\delta s^\varepsilon}\Big] \\
&\quad \pm \frac{1}{\sqrt{\mathcal{D}^\varepsilon}}\,\mathrm{Re}\Big[2B^\varepsilon\big(\overline{v^i_\varepsilon}\,\delta^2 v^\varepsilon_i\big) - 2C^\varepsilon\big(v^i_\varepsilon\,\delta^2 v^\varepsilon_i\big) + 2\big(B^\varepsilon\,\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta^2 s^\varepsilon \\
&\qquad\qquad + 2\Big(s^\varepsilon\big(\overline{v^i_\varepsilon}\,\delta v^\varepsilon_i\big) + \overline{s^\varepsilon}\big(v^i_\varepsilon\,\delta v^\varepsilon_i\big)\Big)\overline{\delta s^\varepsilon} \\
&\qquad\qquad\quad - \big(v^i_\varepsilon\,\delta v^\varepsilon_j\big)\big(\overline{v^i_\varepsilon}\,\overline{\delta v^\varepsilon_i}\big) + \big(v^i_\varepsilon\,\overline{\delta v^\varepsilon_i}\big)\big(\overline{v^j_\varepsilon}\,\delta v^\varepsilon_j\big) - C^\varepsilon\big(\delta v^k_\varepsilon\,\delta v^\varepsilon_k\big) + B^\varepsilon\big(\delta v^k_\varepsilon\,\overline{\delta v^\varepsilon_k}\big)\Big] \\
&\quad \mp \frac{1}{(\mathcal{D}^\varepsilon)^{3/2}}\,\mathrm{Re}\Big[(C^\varepsilon)^2\big(v^k_\varepsilon\,\delta v^\varepsilon_k\big)^2 - 2B^\varepsilon C^\varepsilon\big(v^k_\varepsilon\,\delta v^\varepsilon_k\big)\big(\overline{v^k_\varepsilon}\,\delta v^\varepsilon_k\big) - 2B^\varepsilon C^\varepsilon\big(v^k_\varepsilon\,\delta v^\varepsilon_k\big)\big(v^k_\varepsilon\,\overline{\delta v^\varepsilon_k}\big) \\
&\qquad\qquad + (B^\varepsilon)^2\big(v^k_\varepsilon\,\delta v^\varepsilon_k\big)\big(\overline{v^k_\varepsilon}\,\overline{\delta v^\varepsilon_k}\big) + C^\varepsilon\,\overline{C^\varepsilon}\big(\overline{v^k_\varepsilon}\,\delta v^\varepsilon_k\big)^2 + (B^\varepsilon)^2\big(\overline{v^k_\varepsilon}\,\delta v^\varepsilon_k\big)\big(v^k_\varepsilon\,\overline{\delta v^\varepsilon_k}\big) \\
&\qquad\qquad - 2C^\varepsilon\big(B^\varepsilon\,\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\big(v^k_\varepsilon\,\delta v^\varepsilon_k\big)\delta s^\varepsilon + 2C^\varepsilon\big(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon}\,\overline{s^\varepsilon}\big)\big(\overline{v^k_\varepsilon}\,\delta v^\varepsilon_k\big)\delta s^\varepsilon
\end{aligned}
$$

$$+ 2B^\varepsilon \big(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)(v_\varepsilon^k \delta\overline{v_k^\varepsilon})\delta s^\varepsilon - 2B^\varepsilon \big(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)(v_\varepsilon^k \delta v_k^\varepsilon)\delta\overline{s^\varepsilon}$$
$$+ C^\varepsilon \big(|(v^\varepsilon)^2|^2 - (|v^\varepsilon|^2)^2\big)(\delta s^\varepsilon)^2 + B^\varepsilon \big(|(v^\varepsilon)^2|^2 - (|v^\varepsilon|^2)^2\big)\delta s^\varepsilon \delta\overline{s^\varepsilon}\Big] \quad \text{(B.11)}$$

where B^ε and C^ε as well as the discriminant $\mathcal{D}^\varepsilon$ are the functions introduced in Definition 3.3.3.

Proof. Following the approach by Kato[73, Ch. 2, § 2], the second variation of the eigenvalues is given by

$$\delta^2\lambda_\pm^\varepsilon(x,y) = \frac{1}{2}\,\text{Tr}\left[F_\pm^\varepsilon(x,y)\delta^2 A^\varepsilon(x,y) + \frac{F_\pm^\varepsilon(x,y)\delta A^\varepsilon F_\mp^\varepsilon(x,y)\delta A^\varepsilon}{\lambda_\pm^\varepsilon(x,y) - \lambda_\mp^\varepsilon(x,y)}\right] \tag{B.12}$$

where the prefactor $\frac{1}{2}$ accounts for the twofold degeneracy of the unperturbed eigenvalues $\lambda_\pm^\varepsilon(x,y)$. Suppressing arguments and making use of (3.16) which allows to turn the difference of the eigenvalues into $\lambda_\pm^\varepsilon(x,y) - \lambda_\mp^\varepsilon(x,y) = \pm 2\sqrt{\mathcal{D}^\varepsilon}$, the above formula simplifies to

$$\delta^2\lambda_\pm^\varepsilon = \frac{1}{2}\,\text{Tr}\left[F_\pm^\varepsilon \delta^2 A^\varepsilon \pm \frac{F_\pm^\varepsilon \delta A^\varepsilon F_\mp^\varepsilon \delta A^\varepsilon}{2\sqrt{\mathcal{D}^\varepsilon}}\right] \tag{B.13}$$

To keep the calculations as clear and structured as possible, we first evaluate the term containing $\delta^2 A^\varepsilon$ (which parallels the discussion in Item 1 in the proof of Lemma 3.3.7) and subsequently turn to the second term which involves δA^ε twice. To evaluate the latter term, we subdivide the expressions in manageable parts which can be simplified using the results from Proposition B.1.1 and B.1.4.

(1) Evaluation of the first term in (B.13) (= one occurrence of $\delta^2 A^\varepsilon$)

$$\begin{aligned}
&\text{Tr}\left[F_\pm^\varepsilon \delta^2 A^\varepsilon\right] = \\
&\quad = \text{Tr}\Big[\big(F_{\pm,\text{s}}^\varepsilon \text{id}_{\mathbb{C}^4} + F_{\pm,i}^\varepsilon \gamma^i + F_{\pm,ij}^\varepsilon[\gamma^i,\gamma^j]\big)\big(\delta^2 A_\text{s}^\varepsilon \text{id}_{\mathbb{C}^4} + \delta^2 A_k^\varepsilon \gamma^k + \delta^2 A_{kl}^\varepsilon[\gamma^k \gamma^l]\big)\Big] \\
&\quad = F_{\pm,\text{s}}^\varepsilon \delta^2 A_\text{s}^\varepsilon\,\text{Tr}\left[\text{id}_{\mathbb{C}^4}\right] + F_{\pm,\text{s}}^\varepsilon \delta^2 A_{kl}^\varepsilon\,\text{Tr}\left[[\gamma^k,\gamma^l]\right] + F_{\pm,i}^\varepsilon \delta^2 A_k^\varepsilon\,\text{Tr}\left[\gamma^i\gamma^k\right] \\
&\qquad\qquad + F_{\pm,ij}^\varepsilon \delta^2 A_\text{s}^\varepsilon\,\text{Tr}\left[[\gamma^i,\gamma^j]\right] + F_{\pm,ij}^\varepsilon \delta^2 A_{kl}^\varepsilon\,\text{Tr}\left[[\gamma^i,\gamma^j][\gamma^k,\gamma^l]\right] \\
&\quad \overset{\text{(B.1a)}}{\underset{\text{(B.3c)}}{=}} 4F_{\pm,\text{s}}^\varepsilon \delta^2 A_\text{s}^\varepsilon + 4\eta^{ik} F_{\pm,i}^\varepsilon \delta^2 A_k^\varepsilon + 16\big(-\eta^{ik}\eta^{jl} + \eta^{il}\eta^{jk}\big)F_{\pm,ij}^\varepsilon \delta^2 A_{kl}^\varepsilon
\end{aligned}$$

Inserting the components of $F_\pm^\varepsilon$ from (3.18) as well as of $\delta^2 A^\varepsilon$ from (3.21) we find

$$\begin{aligned}
\ldots &\overset{\text{(3.18)}}{\underset{\text{(3.21)}}{=}} 2\,\text{Re}\,\big(2(\overline{v_\varepsilon^i}\delta^2 v_i^\varepsilon) + 2\overline{s^\varepsilon}\delta^2 s^\varepsilon + (\delta v_\varepsilon^i \delta\overline{v_i^\varepsilon}) + \delta s^\varepsilon \delta\overline{s^\varepsilon}\big) \\
&\qquad \pm 4\frac{\text{Re}(v_\varepsilon^i \overline{s^\varepsilon})}{\sqrt{\mathcal{D}^\varepsilon}} \cdot 2\,\text{Re}\,\big(\overline{s^\varepsilon}\delta^2 v_i^\varepsilon + \overline{v_i^\varepsilon}\delta^2 s^\varepsilon + \delta v_i^\varepsilon \delta\overline{s^\varepsilon}\big) \\
&\qquad \pm 4\frac{v_i^\varepsilon \overline{v_j^\varepsilon}}{\sqrt{\mathcal{D}^\varepsilon}}\big(-\eta^{ik}\eta^{jl} + \eta^{il}\eta^{jk}\big) \cdot \frac{1}{2}\big(\delta^2 v_k^\varepsilon \overline{v_l^\varepsilon} + v_k^\varepsilon \delta^2 \overline{v_l^\varepsilon} + \delta v_k^\varepsilon \delta\overline{v_l^\varepsilon}\big) \\
&= 2\,\text{Re}\,\big(2(\overline{v_\varepsilon^i}\delta^2 v_i^\varepsilon) + 2\overline{s^\varepsilon}\delta^2 s^\varepsilon + (\delta v_\varepsilon^i \delta\overline{v_i^\varepsilon}) + \delta s^\varepsilon \delta\overline{s^\varepsilon}\big) \\
&\qquad \pm \frac{4}{\sqrt{\mathcal{D}^\varepsilon}}\,\text{Re}\,\Big((\overline{s^\varepsilon})^2(v_\varepsilon^i \delta^2 v_i^\varepsilon) + |v^\varepsilon|^2 \overline{s^\varepsilon}\delta^2 s^\varepsilon + \overline{s^\varepsilon}(v_\varepsilon^i \delta v_i^\varepsilon)\delta\overline{s^\varepsilon} \\
&\qquad\qquad + |s^\varepsilon|^2(\overline{v_\varepsilon^i}\delta^2 v_i^\varepsilon) + (\overline{v^\varepsilon})^2 s^\varepsilon \delta^2 s^\varepsilon + s^\varepsilon(\overline{v_\varepsilon^i}\delta v_i^\varepsilon)\delta\overline{s^\varepsilon}\Big) \\
&\qquad \pm \frac{2}{\sqrt{\mathcal{D}^\varepsilon}}\Big(-(v_\varepsilon^i \delta^2 v_i^\varepsilon)(\overline{v^\varepsilon})^2 - (v_\varepsilon^i \delta v_i^\varepsilon)(\overline{v_\varepsilon^j}\delta\overline{v_j^\varepsilon}) - (v^\varepsilon)^2(\overline{v_\varepsilon^i}\delta^2\overline{v_i^\varepsilon}) \\
&\qquad\qquad + |v^\varepsilon|^2(\overline{v_\varepsilon^i}\delta^2 v_i^\varepsilon) + (v_\varepsilon^i \delta\overline{v_i^\varepsilon})(\overline{v_\varepsilon^j}\delta v_j^\varepsilon) + |v^\varepsilon|^2(v_\varepsilon^i \delta^2\overline{v_i^\varepsilon})\Big)
\end{aligned}$$

Collecting terms and forming real parts yields

$$\cdots = 2\,\text{Re}\left[2(\overline{v_\varepsilon^i}\delta^2 v_i^\varepsilon) + 2\overline{s^\varepsilon}\delta^2 s^\varepsilon + (\delta v_\varepsilon^i \delta\overline{v_i^\varepsilon}) + \delta s^\varepsilon \delta\overline{s^\varepsilon}\right]$$

$$\pm \frac{2}{\sqrt{\mathfrak{D}^\varepsilon}} \operatorname{Re} \Big[2\big((\overline{s^\varepsilon})^2 - (\overline{v^\varepsilon})^2\big)(v^i_\varepsilon \delta^2 v^\varepsilon_i) + 2(|s^\varepsilon|^2 + |v^\varepsilon|^2)(\overline{v^i_\varepsilon}\delta^2 v^\varepsilon_i) + 2\big(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta^2 s^\varepsilon \\ + 2\big(s^\varepsilon(\overline{v^i_\varepsilon}\delta v^\varepsilon_i) + \overline{s^\varepsilon}(v^i_\varepsilon \delta v^\varepsilon_i)\big)\delta\overline{s^\varepsilon} - (v^i_\varepsilon \delta v^\varepsilon_i)(\overline{v^j_\varepsilon}\delta\overline{v^\varepsilon_j}) + (v^i_\varepsilon \delta\overline{v^\varepsilon_i})(\overline{v^j_\varepsilon}\delta v^\varepsilon_j)\Big]$$

Expressing everything in terms of $B^\varepsilon \overset{(3.15)}{=} |v^\varepsilon|^2 + |s^\varepsilon|^2$ and $C^\varepsilon \overset{(3.15)}{=} (\overline{v^\varepsilon})^2 - (\overline{s^\varepsilon})^2$ finally results in

$$\begin{aligned} &\operatorname{Tr}\big[F^\varepsilon_\pm \delta^2 A^\varepsilon\big] = \\ &\quad = 2\operatorname{Re}\Big[2(\overline{v^i_\varepsilon}\delta^2 v^\varepsilon_i) + 2\overline{s^\varepsilon}\delta^2 s^\varepsilon + (\delta v^i_\varepsilon \delta\overline{v^\varepsilon_i}) + \delta s^\varepsilon \delta\overline{s^\varepsilon}\Big] \\ &\qquad \pm \frac{2}{\sqrt{\mathfrak{D}^\varepsilon}} \operatorname{Re}\Big[2B^\varepsilon(\overline{v^i_\varepsilon}\delta^2 v^\varepsilon_i) - 2C^\varepsilon(v^i_\varepsilon \delta^2 v^\varepsilon_i) + 2\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta^2 s^\varepsilon \\ &\qquad\quad + 2\big(s^\varepsilon(\overline{v^i_\varepsilon}\delta v^\varepsilon_i) + \overline{s^\varepsilon}(v^i_\varepsilon\delta v^\varepsilon_i)\big)\delta\overline{s^\varepsilon} - (v^i_\varepsilon \delta v^\varepsilon_j)(\overline{v^i_\varepsilon}\delta\overline{v^\varepsilon_i}) + (v^i_\varepsilon\delta\overline{v^\varepsilon_i})(\overline{v^j_\varepsilon}\delta v^\varepsilon_j)\Big] \end{aligned} \tag{B.14}$$

(2) Evaluation of the second term in (B.13) (= two occurrences of δA^ε)
In order to evaluate the second term in (B.13), we first simplify the expression structure-wise by inserting the decompositions of the spectral projectors and the variation of the regularized closed chain from Lemma 3.3.5 and Lemma 3.3.6. Only afterwards, in a second step, we insert the explicit expressions for the components of the variation of the regularized closed chain.

(a) Inserting the Decomposition of $F^\varepsilon_\pm$
Inserting the decompositions of the spectral projector $F^\varepsilon_\pm$ as given in Lemma 3.3.5, the second term in (B.13) becomes

$$\begin{aligned} &\operatorname{Tr}\Big[\underbrace{F^\varepsilon_\pm}_{ij}\,\underbrace{\delta A^\varepsilon}_{kl}\,\underbrace{F^\varepsilon_\mp}_{mn}\,\underbrace{\delta A^\varepsilon}_{pq}\Big] = \\ &= \operatorname{Tr}\Big[\big(F^\varepsilon_{\pm,s}\mathrm{id}_{\mathbb{C}^4} + F^\varepsilon_{\pm,i}\gamma^i + F^\varepsilon_{\pm,ij}[\gamma^i,\gamma^j]\big)\delta A^\varepsilon\big(F^\varepsilon_{\mp,s}\mathrm{id}_{\mathbb{C}^4} + F^\varepsilon_{\mp,m}\gamma^m + F^\varepsilon_{\mp,mn}[\gamma^m,\gamma^n]\big)\delta A^\varepsilon\Big] \\ &= F^\varepsilon_{\pm,s}F^\varepsilon_{\mp,s}\operatorname{Tr}\big[\delta A^\varepsilon\delta A^\varepsilon\big] + F^\varepsilon_{\pm,s}F^\varepsilon_{\mp,m}\operatorname{Tr}\big[\delta A^\varepsilon\gamma^m\delta A^\varepsilon\big] \\ &\qquad + F^\varepsilon_{\pm,s}F^\varepsilon_{\mp,mn}\operatorname{Tr}\big[\delta A^\varepsilon[\gamma^m,\gamma^n]\delta A^\varepsilon\big] \\ &\quad + F^\varepsilon_{\pm,i}F^\varepsilon_{\mp,s}\operatorname{Tr}\big[\gamma^i\delta A^\varepsilon\delta A^\varepsilon\big] + F^\varepsilon_{\pm,i}F^\varepsilon_{\mp,m}\operatorname{Tr}\big[\gamma^i\delta A^\varepsilon\gamma^m\delta A^\varepsilon\big] \\ &\qquad + F^\varepsilon_{\pm,i}F^\varepsilon_{\mp,mn}\operatorname{Tr}\big[\gamma^i\delta A^\varepsilon[\gamma^m,\gamma^n]\delta A^\varepsilon\big] \\ &\quad + F^\varepsilon_{\pm,ij}F^\varepsilon_{\mp,s}\operatorname{Tr}\big[[\gamma^i,\gamma^j]\delta A^\varepsilon\delta A^\varepsilon\big] + F^\varepsilon_{\pm,ij}F^\varepsilon_{\mp,m}\operatorname{Tr}\big[[\gamma^i,\gamma^j]\delta A^\varepsilon\gamma^m\delta A^\varepsilon\big] \\ &\qquad + F^\varepsilon_{\pm,ij}F^\varepsilon_{\mp,mn}\operatorname{Tr}\big[[\gamma^i,\gamma^j]\delta A^\varepsilon[\gamma^m,\gamma^n]\delta A^\varepsilon\big] \\ &\overset{(3.18)}{=} \frac{1}{4}\operatorname{Tr}\big[\delta A^\varepsilon\delta A^\varepsilon\big] \mp \frac{v^\varepsilon_m\overline{s^\varepsilon} + \overline{v^\varepsilon_m}s^\varepsilon}{4\sqrt{\mathfrak{D}^\varepsilon}}\operatorname{Tr}\big[\delta A^\varepsilon\gamma^m\delta A^\varepsilon\big] \mp \frac{v^\varepsilon_m\overline{v^\varepsilon_n}}{8\sqrt{\mathfrak{D}^\varepsilon}}\operatorname{Tr}\big[\delta A^\varepsilon[\gamma^m,\gamma^n]\delta A^\varepsilon\big] \\ &\quad \pm \frac{v^\varepsilon_i\overline{s^\varepsilon} + \overline{v^\varepsilon_i}s^\varepsilon}{4\sqrt{\mathfrak{D}^\varepsilon}}\operatorname{Tr}\big[\gamma^i\delta A^\varepsilon\delta A^\varepsilon\big] - \frac{(v^\varepsilon_i\overline{s^\varepsilon} + \overline{v^\varepsilon_i}s^\varepsilon)(v^\varepsilon_m\overline{s^\varepsilon} + \overline{v^\varepsilon_m}s^\varepsilon)}{4\mathfrak{D}^\varepsilon}\operatorname{Tr}\big[\gamma^i\delta A^\varepsilon\gamma^m\delta A^\varepsilon\big] \\ &\qquad - \frac{(v^\varepsilon_i\overline{s^\varepsilon} + \overline{v^\varepsilon_i}s^\varepsilon)v^\varepsilon_m\overline{v^\varepsilon_n}}{8\mathfrak{D}^\varepsilon}\operatorname{Tr}\big[\gamma^i\delta A^\varepsilon[\gamma^m,\gamma^n]\delta A^\varepsilon\big] \\ &\quad \pm \frac{v^\varepsilon_i\overline{v^\varepsilon_j}}{8\sqrt{\mathfrak{D}^\varepsilon}}\operatorname{Tr}\big[[\gamma^i,\gamma^j]\delta A^\varepsilon\delta A^\varepsilon\big] - \frac{v^\varepsilon_i\overline{v^\varepsilon_j}(v^\varepsilon_m\overline{s^\varepsilon} + \overline{v^\varepsilon_m}s^\varepsilon)}{8\mathfrak{D}^\varepsilon}\operatorname{Tr}\big[[\gamma^i,\gamma^j]\delta A^\varepsilon\gamma^m\delta A^\varepsilon\big] \\ &\qquad - \frac{v^\varepsilon_i\overline{v^\varepsilon_j}v^\varepsilon_m\overline{v^\varepsilon_n}}{16\mathfrak{D}^\varepsilon}\operatorname{Tr}\big[[\gamma^i,\gamma^j]\delta A^\varepsilon[\gamma^m,\gamma^n]\delta A^\varepsilon\big] \\ &= \frac{1}{4}\operatorname{Tr}\big[\delta A^\varepsilon\delta A^\varepsilon\big] - \frac{(v^\varepsilon_i\overline{s^\varepsilon} + \overline{v^\varepsilon_i}s^\varepsilon)(v^\varepsilon_m\overline{s^\varepsilon} + \overline{v^\varepsilon_m}s^\varepsilon)}{4\mathfrak{D}^\varepsilon}\operatorname{Tr}\big[\gamma^i\delta A^\varepsilon\gamma^m\delta A^\varepsilon\big] \end{aligned}$$

$$- \frac{(v_i^\varepsilon \overline{s^\varepsilon} + \overline{v_i^\varepsilon} s^\varepsilon) v_m^\varepsilon \overline{v_n^\varepsilon}}{4\mathfrak{D}^\varepsilon} \operatorname{Tr}\left[\gamma^i \delta A^\varepsilon [\gamma^m, \gamma^n] \delta A^\varepsilon\right] - \frac{v_i^\varepsilon \overline{v_j^\varepsilon} v_m^\varepsilon \overline{v_n^\varepsilon}}{16\mathfrak{D}^\varepsilon} \operatorname{Tr}\left[[\gamma^i, \gamma^j] \delta A^\varepsilon [\gamma^m, \gamma^n] \delta A^\varepsilon\right]$$

(b) Inserting the Decomposition of $\delta A^\varepsilon_\pm$

To further simplify this expression, we insert the decomposition of δA^ε as given in Lemma 3.3.6 which results in

$$\begin{aligned}
&\operatorname{Tr}\Big(\underbrace{F^\varepsilon_\pm}_{ij} \underbrace{\delta A^\varepsilon}_{kl} \underbrace{F^\varepsilon_\mp}_{mn} \underbrace{\delta A^\varepsilon}_{pq} \Big) = \\
&= \frac{1}{4}\Big\{ \delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{\mathrm{s}} \operatorname{Tr}[\mathrm{id}_{\mathbb{C}^4}] + \delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{pq} \operatorname{Tr}\left[[\gamma^p, \gamma^q]\right] + \delta A^\varepsilon_k \delta A^\varepsilon_p \operatorname{Tr}\left[\gamma^k \gamma^p\right] \\
&\qquad + \delta A^\varepsilon_{kl} \delta A^\varepsilon_{\mathrm{s}} \operatorname{Tr}\left[[\gamma^k, \gamma^l]\right] + \delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq} \operatorname{Tr}\left[[\gamma^k, \gamma^l][\gamma^p, \gamma^q]\right] \Big\} \\
&\quad - \frac{(v_i^\varepsilon \overline{s^\varepsilon} + \overline{v_i^\varepsilon} s^\varepsilon)(v_m^\varepsilon \overline{s^\varepsilon} + \overline{v_m^\varepsilon} s^\varepsilon)}{4\mathfrak{D}^\varepsilon} \times \\
&\quad \times \Big\{ \delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{\mathrm{s}} \operatorname{Tr}\left[\gamma^i \gamma^m\right] + \delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{pq} \operatorname{Tr}\left[\gamma^i \gamma^m [\gamma^p, \gamma^q]\right] + \delta A^\varepsilon_k \delta A^\varepsilon_p \operatorname{Tr}\left[\gamma^i \gamma^k \gamma^m \gamma^p\right] \\
&\qquad + \delta A^\varepsilon_{kl} \delta A^\varepsilon_{\mathrm{s}} \operatorname{Tr}\left[\gamma^i [\gamma^k, \gamma^l] \gamma^m\right] + \delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq} \operatorname{Tr}\left[\gamma^i [\gamma^k, \gamma^l] \gamma^m [\gamma^p, \gamma^q]\right] \Big\} \\
&\quad - \frac{(v_i^\varepsilon \overline{s^\varepsilon} + \overline{v_i^\varepsilon} s^\varepsilon) v_m^\varepsilon \overline{v_n^\varepsilon}}{4\mathfrak{D}^\varepsilon} \times \\
&\quad \times \Big\{ \delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_p \operatorname{Tr}\left[\gamma^i [\gamma^m, \gamma^n] \gamma^p\right] + \delta A^\varepsilon_k \delta A^\varepsilon_{\mathrm{s}} \operatorname{Tr}\left[\gamma^i \gamma^k [\gamma^m, \gamma^n]\right] \\
&\qquad + \delta A^\varepsilon_k \delta A^\varepsilon_{pq} \operatorname{Tr}\left[\gamma^i \gamma^k [\gamma^m, \gamma^n][\gamma^p, \gamma^q]\right] + \delta A^\varepsilon_{kl} \delta A^\varepsilon_p \operatorname{Tr}\left[\gamma^i [\gamma^k, \gamma^l][\gamma^m, \gamma^n] \gamma^p\right] \Big\} \\
&\quad - \frac{v_i^\varepsilon \overline{v_j^\varepsilon} v_m^\varepsilon \overline{v_n^\varepsilon}}{16\mathfrak{D}^\varepsilon} \Big\{ \delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{\mathrm{s}} \operatorname{Tr}\left[[\gamma^i, \gamma^j][\gamma^m, \gamma^n]\right] + \delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{pq} \operatorname{Tr}\left[[\gamma^i, \gamma^j][\gamma^m, \gamma^n][\gamma^p, \gamma^q]\right] \\
&\qquad + \delta A^\varepsilon_k \delta A^\varepsilon_p \operatorname{Tr}\left[[\gamma^i, \gamma^j] \gamma^k [\gamma^m, \gamma^n] \gamma^p\right] + \delta A^\varepsilon_{kl} \delta A^\varepsilon_{\mathrm{s}} \operatorname{Tr}\left[[\gamma^i, \gamma^j][\gamma^k, \gamma^l][\gamma^m, \gamma^n]\right] \\
&\qquad + \delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq} \operatorname{Tr}\left[[\gamma^i, \gamma^j][\gamma^k, \gamma^l][\gamma^m, \gamma^n][\gamma^p, \gamma^q]\right] \Big\} \\
&= \frac{1}{4}\Big\{ \delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{\mathrm{s}} \operatorname{Tr}[\mathrm{id}_{\mathbb{C}^4}] + 2\delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{pq} \operatorname{Tr}\left[[\gamma^p, \gamma^q]\right] \\
&\qquad + \delta A^\varepsilon_k \delta A^\varepsilon_p \operatorname{Tr}\left[\gamma^k \gamma^p\right] + \delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq} \operatorname{Tr}\left[[\gamma^k, \gamma^l][\gamma^p, \gamma^q]\right] \Big\} \\
&\quad - \frac{(v_i^\varepsilon \overline{s^\varepsilon} + \overline{v_i^\varepsilon} s^\varepsilon)(v_m^\varepsilon \overline{s^\varepsilon} + \overline{v_m^\varepsilon} s^\varepsilon)}{4\mathfrak{D}^\varepsilon} \times \\
&\quad \times \Big\{ \delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{\mathrm{s}} \operatorname{Tr}\left[\gamma^i \gamma^m\right] + 2\delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{pq} \operatorname{Tr}\left[\gamma^i \gamma^m [\gamma^p, \gamma^q]\right] \\
&\qquad + \delta A^\varepsilon_k \delta A^\varepsilon_p \operatorname{Tr}\left[\gamma^i \gamma^k \gamma^m \gamma^p\right] + \delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq} \operatorname{Tr}\left[\gamma^i [\gamma^k, \gamma^l] \gamma^m [\gamma^p, \gamma^q]\right] \Big\} \\
&\quad - \frac{(v_i^\varepsilon \overline{s^\varepsilon} + \overline{v_i^\varepsilon} s^\varepsilon) v_m^\varepsilon \overline{v_n^\varepsilon}}{4\mathfrak{D}^\varepsilon} \Big\{ 2\delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_k \eta^{ik} \operatorname{Tr}\left[[\gamma^m, \gamma^n]\right] + \delta A^\varepsilon_k \delta A^\varepsilon_{pq} \operatorname{Tr}\left[\gamma^i \gamma^k [\gamma^m, \gamma^n][\gamma^p, \gamma^q]\right] \\
&\qquad + \delta A^\varepsilon_{kl} \delta A^\varepsilon_p \operatorname{Tr}\left[\gamma^i [\gamma^k, \gamma^l][\gamma^m, \gamma^n] \gamma^p\right] \Big\} \\
&\quad - \frac{v_i^\varepsilon \overline{v_j^\varepsilon} v_m^\varepsilon \overline{v_n^\varepsilon}}{16\mathfrak{D}^\varepsilon} \Big\{ \delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{\mathrm{s}} \operatorname{Tr}\left[[\gamma^i, \gamma^j][\gamma^m, \gamma^n]\right] + 2\delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{pq} \operatorname{Tr}\left[[\gamma^i, \gamma^j][\gamma^m, \gamma^n][\gamma^p, \gamma^q]\right] \\
&\qquad + \delta A^\varepsilon_k \delta A^\varepsilon_p \operatorname{Tr}\left[[\gamma^i, \gamma^j] \gamma^k [\gamma^m, \gamma^n] \gamma^p\right] \\
&\qquad + \delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq} \operatorname{Tr}\left[[\gamma^i, \gamma^j][\gamma^k, \gamma^l][\gamma^m, \gamma^n][\gamma^p, \gamma^q]\right] \Big\}
\end{aligned} \tag{B.15}$$

In order not to loose track, we split the expression and evaluate the four terms separately.

(i) First Term in (B.15)

$$(\mathbf{1}) = \frac{1}{4}\Big\{\delta A^\varepsilon_{\mathrm{s}}\delta A^\varepsilon_{\mathrm{s}}\,\mathrm{Tr}[\mathrm{id}_{\mathbb{C}^4}] + 2\delta A^\varepsilon_{\mathrm{s}}\delta A^\varepsilon_{pq}\underbrace{\mathrm{Tr}\big[[\gamma^p,\gamma^q]\big]}_{\to 0} + \delta A^\varepsilon_k\delta A^\varepsilon_p\underbrace{\mathrm{Tr}\big[\gamma^k\gamma^p\big]}_{\text{(B.1a)}} + \delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}\underbrace{\mathrm{Tr}\big[[\gamma^k,\gamma^l][\gamma^p,\gamma^q]\big]}_{\text{(B.3c)}}\Big\}$$
$$= \delta A^\varepsilon_{\mathrm{s}}\delta A^\varepsilon_{\mathrm{s}} + \delta A^\varepsilon_k\delta A^\varepsilon_p\eta^{kp} + 4\delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big) \tag{B.16a}$$

(ii) Second Term in (B.15)

$$(\mathbf{2}) = -\frac{(v^\varepsilon_i\overline{s^\varepsilon} + \overline{v^\varepsilon_i}s^\varepsilon)(v^\varepsilon_m\overline{s^\varepsilon} + \overline{v^\varepsilon_m}s^\varepsilon)}{4\mathfrak{D}^\varepsilon}\times$$
$$\times\Big\{\delta A^\varepsilon_{\mathrm{s}}\delta A^\varepsilon_{\mathrm{s}}\underbrace{\mathrm{Tr}\big[\gamma^i\gamma^m\big]}_{\text{(B.1a)}} + 2\delta A^\varepsilon_{\mathrm{s}}\delta A^\varepsilon_{pq}\underbrace{\mathrm{Tr}\big[\gamma^i\gamma^m[\gamma^p,\gamma^q]\big]}_{\text{(B.3b)}} + \delta A^\varepsilon_k\delta A^\varepsilon_p\underbrace{\mathrm{Tr}\big[\gamma^i\gamma^k\gamma^m\gamma^p\big]}_{\text{(B.3a)}} + \delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}\underbrace{\mathrm{Tr}\big[\gamma^i[\gamma^k,\gamma^l]\gamma^m[\gamma^p,\gamma^q]\big]}_{\text{(B.7c)}}\Big\}$$
$$= -\frac{(v^\varepsilon_i\overline{s^\varepsilon} + \overline{v^\varepsilon_i}s^\varepsilon)(v^\varepsilon_m\overline{s^\varepsilon} + \overline{v^\varepsilon_m}s^\varepsilon)}{4\mathfrak{D}^\varepsilon}\times$$
$$\times\Big\{4\delta A^\varepsilon_{\mathrm{s}}\delta A^\varepsilon_{\mathrm{s}}\eta^{im} + 16\delta A^\varepsilon_{\mathrm{s}}\delta A^\varepsilon_{pq}\underbrace{\big(-\eta^{ip}\eta^{mq} + \eta^{iq}\eta^{mp}\big)}_{\to 0} + 4\delta A^\varepsilon_k\delta A^\varepsilon_p\big(\underbrace{\eta^{ik}\eta^{mp}}_{\to(1)} - \eta^{im}\eta^{kp} + \underbrace{\eta^{ip}\eta^{km}}_{=(1)}\big)$$
$$+ 16\delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}\Big[\eta^{ik}\underbrace{\big(-\eta^{lp}\eta^{mq} + \eta^{lq}\eta^{mp}\big)}_{\to(2)} - \eta^{il}\underbrace{\big(-\eta^{kp}\eta^{mq} + \eta^{kq}\eta^{mp}\big)}_{\to(3)} + \eta^{im}\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big) - \eta^{ip}\underbrace{\big(-\eta^{km}\eta^{lq} + \eta^{kq}\eta^{lm}\big)}_{=(2)} + \eta^{iq}\underbrace{\big(-\eta^{km}\eta^{lp} + \eta^{kp}\eta^{lm}\big)}_{=(3)}\Big]\Big\}$$
$$= -\frac{1}{\mathfrak{D}^\varepsilon}\Big\{\delta A^\varepsilon_{\mathrm{s}}\delta A^\varepsilon_{\mathrm{s}}((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2)$$
$$+ \delta A^\varepsilon_k\delta A^\varepsilon_p\Big[2(v^k_\varepsilon\overline{s^\varepsilon} + \overline{v^k_\varepsilon}s^\varepsilon)(v^p_\varepsilon\overline{s^\varepsilon} + \overline{v^p_\varepsilon}s^\varepsilon) - ((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2)\eta^{kp}\Big]$$
$$+ 4\delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}\Big[2(v^k_\varepsilon\overline{s^\varepsilon} + \overline{v^k_\varepsilon}s^\varepsilon)\big(\underbrace{-\eta^{lp}(v^q_\varepsilon\overline{s^\varepsilon} + \overline{v^q_\varepsilon}s^\varepsilon)}_{\to(4)} + \eta^{lq}(v^p_\varepsilon\overline{s^\varepsilon} + \overline{v^p_\varepsilon}s^\varepsilon)\big)$$
$$- 2(v^l_\varepsilon\overline{s^\varepsilon} + \overline{v^l_\varepsilon}s^\varepsilon)\big(-\eta^{kp}(v^q_\varepsilon\overline{s^\varepsilon} + \overline{v^q_\varepsilon}s^\varepsilon) + \underbrace{\eta^{kq}(v^p_\varepsilon\overline{s^\varepsilon} + \overline{v^p_\varepsilon}s^\varepsilon)}_{=(4)}\big)$$
$$+ ((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2)\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big)\Big]\Big\}$$
$$= -\frac{1}{\mathfrak{D}^\varepsilon}\Big\{\delta A^\varepsilon_{\mathrm{s}}\delta A^\varepsilon_{\mathrm{s}}((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2)$$
$$+ \delta A^\varepsilon_k\delta A^\varepsilon_p\Big[2(v^k_\varepsilon\overline{s^\varepsilon} + \overline{v^k_\varepsilon}s^\varepsilon)(v^p_\varepsilon\overline{s^\varepsilon} + \overline{v^p_\varepsilon}s^\varepsilon) - ((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2)\eta^{kp}\Big]$$
$$+ 4\delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}\Big[2(v^k_\varepsilon\overline{s^\varepsilon} + \overline{v^k_\varepsilon}s^\varepsilon)(v^p_\varepsilon\overline{s^\varepsilon} + \overline{v^p_\varepsilon}s^\varepsilon)\eta^{lq} + 2(v^l_\varepsilon\overline{s^\varepsilon} + \overline{v^l_\varepsilon}s^\varepsilon)(v^q_\varepsilon\overline{s^\varepsilon} + \overline{v^q_\varepsilon}s^\varepsilon)\eta^{kp}$$
$$- 4(v^k_\varepsilon\overline{s^\varepsilon} + \overline{v^k_\varepsilon}s^\varepsilon)(v^q_\varepsilon\overline{s^\varepsilon} + \overline{v^q_\varepsilon}s^\varepsilon)\eta^{lp}$$
$$+ ((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2)\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big)\Big]\Big\} \tag{B.16b}$$

(iii) Third Term in (B.15)

$$
\begin{aligned}
(\mathbf{3}) = &-\frac{(v_i^\varepsilon \overline{s^\varepsilon} + \overline{v_i^\varepsilon} s^\varepsilon) v_m^\varepsilon \overline{v_n^\varepsilon}}{4\mathcal{D}^\varepsilon} \times \\
&\times \Big\{ 2\delta A_s^\varepsilon \delta A_k^\varepsilon \eta^{ik} \cancelto{0}{\operatorname{Tr}\big[[\gamma^m, \gamma^n]\big]} + \delta A_k^\varepsilon \delta A_{pq}^\varepsilon \underbrace{\operatorname{Tr}\big[\gamma^i \gamma^k [\gamma^m, \gamma^n][\gamma^p, \gamma^q]\big]}_{(B.7b)} \\
&\qquad + \delta A_{kl}^\varepsilon \delta A_p^\varepsilon \underbrace{\operatorname{Tr}\big[\gamma^i [\gamma^k, \gamma^l][\gamma^m, \gamma^n]\gamma^p\big]}_{(B.7b)} \Big\}
\end{aligned}
$$

$$
\begin{aligned}
= &-\frac{(v_i^\varepsilon \overline{s^\varepsilon} + \overline{v_i^\varepsilon} s^\varepsilon) v_m^\varepsilon \overline{v_n^\varepsilon}}{4\mathcal{D}^\varepsilon} \times \\
&\times \Big\{ 16\delta A_k^\varepsilon \delta A_{pq}^\varepsilon \Big[\cancelto{(1)}{\eta^{ik}\big(-\eta^{mp}\eta^{nq} + \eta^{mq}\eta^{np}\big)} - \eta^{im}\big(-\cancelto{(2)}{\eta^{kp}\eta^{nq}} + \cancelto{(3)}{\eta^{kq}\eta^{np}}\big) \\
&\qquad + \eta^{in}\big(-\cancelto{(4)}{\eta^{kp}\eta^{mq}} + \cancelto{(5)}{\eta^{kq}\eta^{mp}}\big) - \eta^{ip}\big(\cancelto{(6)}{\eta^{km}\eta^{nq}} - \cancelto{(7)}{\eta^{kn}\eta^{mq}}\big) \\
&\qquad + \eta^{iq}\big(\cancelto{(8)}{\eta^{km}\eta^{np}} - \cancelto{(9)}{\eta^{kn}\eta^{mp}}\big) \Big] \\
&+ 16\delta A_{kl}^\varepsilon \delta A_p^\varepsilon \Big[\cancelto{=(1)}{\eta^{pi}\big(-\eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big)} - \eta^{pk}\big(-\cancelto{=(2)}{\eta^{im}\eta^{ln}} + \cancelto{=(4)}{\eta^{in}\eta^{lm}}\big) \\
&\qquad + \eta^{pl}\big(-\cancelto{=(3)}{\eta^{im}\eta^{kn}} + \cancelto{=(5)}{\eta^{in}\eta^{km}}\big) - \eta^{pm}\big(\cancelto{=(6)}{\eta^{ik}\eta^{ln}} - \cancelto{=(8)}{\eta^{il}\eta^{kn}}\big) \\
&\qquad + \eta^{pn}\big(\cancelto{=(7)}{\eta^{ik}\eta^{lm}} - \cancelto{=(9)}{\eta^{il}\eta^{km}}\big) \Big] \Big\}
\end{aligned}
$$

$$
\begin{aligned}
= -\frac{1}{\mathcal{D}^\varepsilon} \Big\{ & 8\delta A_k^\varepsilon \delta A_{pq}^\varepsilon \Big[(v_\varepsilon^k \overline{s^\varepsilon} + \overline{v_\varepsilon^k} s^\varepsilon)\big(-v_\varepsilon^p \overline{v_\varepsilon^q} + v_\varepsilon^q \overline{v_\varepsilon^p}\big) - \big(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon s^\varepsilon}\big)\big(-\eta^{kp}\overline{v_\varepsilon^q} + \eta^{kq}\overline{v_\varepsilon^p}\big) \\
&+ (B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon)\big(-\eta^{kp} v_\varepsilon^q + \eta^{kq} v_\varepsilon^p\big) \\
&- (v_\varepsilon^p \overline{s^\varepsilon} + \overline{v_\varepsilon^p} s^\varepsilon)\big(v_\varepsilon^k \overline{v_\varepsilon^q} - \overline{v_\varepsilon^k} v_\varepsilon^q\big) + (v_\varepsilon^q \overline{s^\varepsilon} + \overline{v_\varepsilon^q} s^\varepsilon)\big(v_\varepsilon^k \overline{v_\varepsilon^p} - \overline{v_\varepsilon^k} v_\varepsilon^p\big) \Big] \Big\}
\end{aligned} \tag{B.16c}
$$

(iv) Fourth Term in (B.15)

$$
\begin{aligned}
(\mathbf{4}) = &-\frac{v_i^\varepsilon \overline{v_j^\varepsilon} v_m^\varepsilon \overline{v_n^\varepsilon}}{16\mathcal{D}^\varepsilon} \times \\
&\times \Big\{ \delta A_s^\varepsilon \delta A_s^\varepsilon \underbrace{\operatorname{Tr}\big[[\gamma^i, \gamma^j][\gamma^m, \gamma^n]\big]}_{(B.3c)} + 2\delta A_s^\varepsilon \delta A_{pq}^\varepsilon \underbrace{\operatorname{Tr}\big[[\gamma^i, \gamma^j][\gamma^m, \gamma^n][\gamma^p, \gamma^q]\big]}_{(B.7d)} \\
&\quad + \delta A_k^\varepsilon \delta A_p^\varepsilon \underbrace{\operatorname{Tr}\big[[\gamma^i, \gamma^j]\gamma^k[\gamma^m, \gamma^n]\gamma^p\big]}_{(B.7c)} + \delta A_{kl}^\varepsilon \delta A_{pq}^\varepsilon \underbrace{\operatorname{Tr}\big[[\gamma^i, \gamma^j][\gamma^k, \gamma^l][\gamma^m, \gamma^n][\gamma^p, \gamma^q]\big]}_{(B.9b)} \Big\} \\
= &-\frac{v_i^\varepsilon \overline{v_j^\varepsilon} v_m^\varepsilon \overline{v_n^\varepsilon}}{16\mathcal{D}^\varepsilon} \times \\
&\times \Big\{ 16\delta A_s^\varepsilon \delta A_s^\varepsilon \big(-\eta^{im}\eta^{jn} + \eta^{in}\eta^{jm}\big) \\
&\quad + 64\delta A_s^\varepsilon \delta A_{pq}^\varepsilon \Big[-\eta^{im}\big(-\eta^{jp}\eta^{nq} + \eta^{jq}\eta^{np}\big) + \eta^{in}\big(-\eta^{jp}\eta^{mq} + \eta^{jq}\eta^{mp}\big) \\
&\qquad - \eta^{ip}\big(\eta^{jm}\eta^{nq} - \eta^{jn}\eta^{mq}\big) + \eta^{iq}\big(\eta^{jm}\eta^{np} - \eta^{jn}\eta^{mp}\big) \Big]
\end{aligned}
$$

$$
\begin{aligned}
&+16\delta A^\varepsilon_k \delta A^\varepsilon_p \Big[-\eta^{ik}\big(\eta^{jm}\eta^{np} - \eta^{jn}\eta^{mp}\big) + \eta^{im}\big(\eta^{jk}\eta^{np} - \eta^{jn}\eta^{kp} + \eta^{jp}\eta^{kn}\big) \\
&\qquad - \eta^{in}\big(\eta^{jk}\eta^{mp} - \eta^{jm}\eta^{kp} + \eta^{jp}\eta^{km}\big) + \eta^{ip}\big(-\eta^{jm}\eta^{kn} + \eta^{jn}\eta^{km}\big)\Big] \\
&+16\delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq} \Big[-4\eta^{ik}\Big(\eta^{jl}\big(-\eta^{mp}\eta^{nq} + \eta^{mq}\eta^{np}\big) - \eta^{jm}\big(-\eta^{lp}\eta^{nq} + \eta^{lq}\eta^{np}\big) \\
&\qquad + \eta^{jn}\big(-\eta^{lp}\eta^{mq} + \eta^{lq}\eta^{mp}\big) - \eta^{jp}\big(\eta^{lm}\eta^{nq} - \eta^{ln}\eta^{mq}\big) \\
&\qquad + \eta^{jq}\big(\eta^{lm}\eta^{np} - \eta^{ln}\eta^{mp}\big)\Big) \\
&\quad + 4\eta^{il}\Big(\eta^{jk}\big(-\eta^{mp}\eta^{nq} + \eta^{mq}\eta^{np}\big) - \eta^{jm}\big(-\eta^{kp}\eta^{nq} + \eta^{kq}\eta^{np}\big) \\
&\qquad + \eta^{jn}\big(-\eta^{kp}\eta^{mq} + \eta^{kq}\eta^{mp}\big) - \eta^{jp}\big(\eta^{km}\eta^{nq} - \eta^{kn}\eta^{mq}\big) \\
&\qquad + \eta^{jq}\big(\eta^{km}\eta^{np} - \eta^{kn}\eta^{mp}\big)\Big) \\
&\quad - 4\eta^{im}\Big(\eta^{jk}\big(-\eta^{lp}\eta^{nq} + \eta^{lq}\eta^{np}\big) - \eta^{jl}\big(-\eta^{kp}\eta^{nq} + \eta^{kq}\eta^{np}\big) \\
&\qquad + \eta^{jn}\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big) - \eta^{jp}\big(-\eta^{kn}\eta^{lq} + \eta^{kq}\eta^{ln}\big) \\
&\qquad + \eta^{jq}\big(-\eta^{kn}\eta^{lp} + \eta^{kp}\eta^{ln}\big)\Big) \\
&\quad + 4\eta^{in}\Big(\eta^{jk}\big(-\eta^{lp}\eta^{mq} + \eta^{lq}\eta^{mp}\big) - \eta^{jl}\big(-\eta^{kp}\eta^{mq} + \eta^{kq}\eta^{mp}\big) \\
&\qquad + \eta^{jm}\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big) - \eta^{jp}\big(-\eta^{km}\eta^{lq} + \eta^{kq}\eta^{lm}\big) \\
&\qquad + \eta^{jq}\big(-\eta^{km}\eta^{lp} + \eta^{kp}\eta^{lm}\big)\Big) \\
&\quad - 4\eta^{ip}\Big(\eta^{jk}\big(\eta^{lm}\eta^{nq} - \eta^{ln}\eta^{mq}\big) - \eta^{jl}\big(\eta^{km}\eta^{nq} - \eta^{kn}\eta^{mq}\big) \\
&\qquad + \eta^{jm}\big(-\eta^{kn}\eta^{lq} + \eta^{kq}\eta^{ln}\big) - \eta^{jn}\big(-\eta^{km}\eta^{lq} + \eta^{kq}\eta^{lm}\big) \\
&\qquad + \eta^{jq}\big(-\eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big)\Big) \\
&\quad + 4\eta^{iq}\Big(\eta^{jk}\big(\eta^{lm}\eta^{np} - \eta^{ln}\eta^{mp}\big) - \eta^{jl}\big(\eta^{km}\eta^{np} - \eta^{kn}\eta^{mp}\big) \\
&\qquad + \eta^{jm}\big(-\eta^{kn}\eta^{lp} + \eta^{kp}\eta^{ln}\big) - \eta^{jn}\big(-\eta^{km}\eta^{lp} + \eta^{kp}\eta^{lm}\big) \\
&\qquad + \eta^{jp}\big(-\eta^{km}\eta^{ln} + \eta^{kn}\eta^{lm}\big)\Big)\Big]\Bigg\}
\end{aligned}
$$

$$
\begin{aligned}
= -\frac{1}{\mathcal{D}^\varepsilon}\Bigg\{ &\delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{\mathrm{s}}\big(-(v^\varepsilon)^2(\overline{v^\varepsilon})^2 + (|v^\varepsilon|^2)^2\big) \\
&+4\delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{pq}\Big[-(v^\varepsilon)^2\big(-\overline{v^p_\varepsilon}\,\overline{v^q_\varepsilon} + \overline{v^q_\varepsilon}\,\overline{v^p_\varepsilon}\big) + |v^\varepsilon|^2\big(-\overline{v^p_\varepsilon}v^q_\varepsilon + \overline{v^q_\varepsilon}v^p_\varepsilon\big) \\
&\qquad - v^p_\varepsilon\big(|v^\varepsilon|^2\overline{v^q_\varepsilon} - (\overline{v^\varepsilon})^2 v^q_\varepsilon\big) + v^q_\varepsilon\big(|v^\varepsilon|^2\overline{v^p_\varepsilon} - (\overline{v^\varepsilon})^2 v^p_\varepsilon\big)\Big] \\
&+\delta A^\varepsilon_k \delta A^\varepsilon_p\Big[-v^k_\varepsilon\big(|v^\varepsilon|^2\overline{v^p_\varepsilon} - (\overline{v^\varepsilon})^2 v^p_\varepsilon\big) + (v^\varepsilon)^2\big(\overline{v^k_\varepsilon}\,\overline{v^p_\varepsilon} - (\overline{v^\varepsilon})^2\eta^{kp} + \overline{v^p_\varepsilon}\,\overline{v^k_\varepsilon}\big) \\
&\qquad - |v^\varepsilon|^2\big(\overline{v^k_\varepsilon}v^p_\varepsilon - |v^\varepsilon|^2\eta^{kp} + \overline{v^p_\varepsilon}v^k_\varepsilon\big) + v^p_\varepsilon\big(-|v^\varepsilon|^2\overline{v^k_\varepsilon} + (\overline{v^\varepsilon})^2 v^k_\varepsilon\big)\Big] \\
&+\delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq}\Big[-4v^k_\varepsilon\Big(\overline{v^l_\varepsilon}\big(-v^p_\varepsilon\overline{v^q_\varepsilon} + v^q_\varepsilon\overline{v^p_\varepsilon}\big) - |v^\varepsilon|^2\big(-\eta^{lp}\overline{v^q_\varepsilon} + \eta^{lq}\overline{v^p_\varepsilon}\big) \\
&\qquad + (\overline{v^\varepsilon})^2\big(-\eta^{lp}v^q_\varepsilon + \eta^{lq}v^p_\varepsilon\big) - \overline{v^p_\varepsilon}\big(v^l_\varepsilon\overline{v^q_\varepsilon} - \overline{v^l_\varepsilon}v^q_\varepsilon\big) + \overline{v^q_\varepsilon}\big(v^l_\varepsilon\overline{v^p_\varepsilon} - \overline{v^l_\varepsilon}v^p_\varepsilon\big)\Big) \\
&\quad + 4v^l_\varepsilon\Big(\overline{v^k_\varepsilon}\big(-v^p_\varepsilon\overline{v^q_\varepsilon} + v^q_\varepsilon\overline{v^p_\varepsilon}\big) - |v^\varepsilon|^2\big(-\eta^{kp}\overline{v^q_\varepsilon} + \eta^{kq}\overline{v^p_\varepsilon}\big) \\
&\qquad + (\overline{v^\varepsilon})^2\big(-\eta^{kp}v^q_\varepsilon + \eta^{kq}v^p_\varepsilon\big) - \overline{v^p_\varepsilon}\big(v^k_\varepsilon\overline{v^q_\varepsilon} - \overline{v^k_\varepsilon}v^q_\varepsilon\big) \\
&\qquad + \overline{v^q_\varepsilon}\big(v^k_\varepsilon\overline{v^p_\varepsilon} - \overline{v^k_\varepsilon}v^p_\varepsilon\big)\Big) \\
&\quad - 4(v^\varepsilon)^2\Big(\overline{v^k_\varepsilon}\big(-\eta^{lp}\overline{v^q_\varepsilon} + \eta^{lq}\overline{v^p_\varepsilon}\big) - \overline{v^l_\varepsilon}\big(-\eta^{kp}\overline{v^q_\varepsilon} + \eta^{kq}\overline{v^p_\varepsilon}\big) \\
&\qquad + (\overline{v^\varepsilon})^2\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big) - \overline{v^p_\varepsilon}\big(-\overline{v^k_\varepsilon}\eta^{lq} + \eta^{kq}\overline{v^l_\varepsilon}\big) \\
&\qquad + \overline{v^q_\varepsilon}\big(-\overline{v^k_\varepsilon}\eta^{lp} + \eta^{kp}\overline{v^l_\varepsilon}\big)\Big)
\end{aligned}
$$

$$
\begin{aligned}
&+ 4|v^\varepsilon|^2 \Big(\overline{v^k_\varepsilon}\big(- \eta^{lp} v^q_\varepsilon + \eta^{lq} v^p_\varepsilon \big) - \overline{v^l_\varepsilon}\big(- \eta^{kp} v^q_\varepsilon + \eta^{kq} v^p_\varepsilon \big) \\
&\qquad + |v^\varepsilon|^2 \big(- \eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp} \big) - \overline{v^p_\varepsilon}\big(- v^k_\varepsilon \eta^{lq} + \eta^{kq} v^l_\varepsilon \big) \\
&\qquad + \overline{v^q_\varepsilon}\big(- v^k_\varepsilon \eta^{lp} + \eta^{kp} v^l_\varepsilon \big) \Big) \\
&- 4 v^p_\varepsilon \Big(\overline{v^k_\varepsilon}\big(v^l_\varepsilon \overline{v^q_\varepsilon} - \overline{v^l_\varepsilon} v^q_\varepsilon \big) - \overline{v^l_\varepsilon}\big(v^k_\varepsilon \overline{v^q_\varepsilon} - \overline{v^k_\varepsilon} v^q_\varepsilon \big) + |v^\varepsilon|^2 \big(- \overline{v^k_\varepsilon} \eta^{lq} + \eta^{kq} \overline{v^l_\varepsilon} \big) \\
&\qquad - (\overline{v^\varepsilon})^2 \big(- v^k_\varepsilon \eta^{lq} + \eta^{kq} v^l_\varepsilon \big) + \overline{v^q_\varepsilon}\big(- v^k_\varepsilon \overline{v^l_\varepsilon} + \overline{v^k_\varepsilon} v^l_\varepsilon \big) \Big) \\
&+ 4 v^q_\varepsilon \Big(\overline{v^k_\varepsilon}\big(v^l_\varepsilon \overline{v^p_\varepsilon} - \overline{v^l_\varepsilon} v^p_\varepsilon \big) - \overline{v^l_\varepsilon}\big(v^k_\varepsilon \overline{v^p_\varepsilon} - \overline{v^k_\varepsilon} v^p_\varepsilon \big) + |v^\varepsilon|^2 \big(- \overline{v^k_\varepsilon} \eta^{lp} + \eta^{kp} \overline{v^l_\varepsilon} \big) \\
&\qquad - (\overline{v^\varepsilon})^2 \big(- v^k_\varepsilon \eta^{lp} + \eta^{kp} v^l_\varepsilon \big) + \overline{v^p_\varepsilon}\big(- v^k_\varepsilon \overline{v^l_\varepsilon} + \overline{v^k_\varepsilon} v^l_\varepsilon \big) \Big) \Big] \Big\}
\end{aligned}
$$

$$
\begin{aligned}
= -\frac{1}{\mathcal{D}^\varepsilon} \Big\{ & \delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{\mathrm{s}} \big(- (v^\varepsilon)^2 (\overline{v^\varepsilon})^2 + (|v^\varepsilon|^2)^2 \big) \\
&+ \delta A^\varepsilon_k \delta A^\varepsilon_p \Big[- 2 v^k_\varepsilon \big(\cancelto{(1)}{|v^\varepsilon|^2 \overline{v^p_\varepsilon}} - (\overline{v^\varepsilon})^2 v^p_\varepsilon \big) + (v^\varepsilon)^2 \big(2\overline{v^k_\varepsilon v^p_\varepsilon} - (\overline{v^\varepsilon})^2 \eta^{kp} \big) \\
&\qquad - |v^\varepsilon|^2 \big(\cancelto{=(1)}{2\overline{v^k_\varepsilon} v^p_\varepsilon} - |v^\varepsilon|^2 \eta^{kp} \big) \Big] \\
&+ \delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq} \Big[- 4 v^k_\varepsilon \Big(4\overline{v^l_\varepsilon}\big(- v^p_\varepsilon \overline{v^q_\varepsilon} + \cancelto{(2)}{v^q_\varepsilon \overline{v^p_\varepsilon}} \big) - 2|v^\varepsilon|^2 \big(- \cancelto{(5)}{\eta^{lp} \overline{v^q_\varepsilon}} + \cancelto{(6)}{\eta^{lq} \overline{v^p_\varepsilon}} \big) \\
&\qquad + 2(\overline{v^\varepsilon})^2 \big(- \cancelto{(7)}{\eta^{lp} v^q_\varepsilon} + \eta^{lq} v^p_\varepsilon \big) \Big) \\
&\quad + 4 v^l_\varepsilon \Big(4\overline{v^k_\varepsilon}\big(- \cancelto{=(2)}{v^p_\varepsilon \overline{v^q_\varepsilon}} + v^q_\varepsilon \overline{v^p_\varepsilon} \big) - 2|v^\varepsilon|^2 \big(- \cancelto{(3)}{\eta^{kp} \overline{v^q_\varepsilon}} + \cancelto{(4)}{\eta^{kq} \overline{v^p_\varepsilon}} \big) \\
&\qquad + 2(\overline{v^\varepsilon})^2 \big(- \eta^{kp} v^q_\varepsilon + \cancelto{=(7)}{\eta^{kq} v^p_\varepsilon} \big) \Big) \\
&\quad - 4 (v^\varepsilon)^2 \Big(2\overline{v^k_\varepsilon}\big(- \eta^{lp} \overline{v^q_\varepsilon} + \eta^{lq} \overline{v^p_\varepsilon} \big) - 2\overline{v^l_\varepsilon}\big(- \eta^{kp} \overline{v^q_\varepsilon} + \eta^{kq} \overline{v^p_\varepsilon} \big) \\
&\qquad + (\overline{v^\varepsilon})^2 \big(- \eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp} \big) \Big) \\
&\quad + 4|v^\varepsilon|^2 \Big(2\overline{v^k_\varepsilon}\big(- \cancelto{=(4)}{\eta^{lp} v^q_\varepsilon} + \cancelto{=(6)}{\eta^{lq} v^p_\varepsilon} \big) - 2\overline{v^l_\varepsilon}\big(- \cancelto{=(3)}{\eta^{kp} v^q_\varepsilon} + \cancelto{=(5)}{\eta^{kq} v^p_\varepsilon} \big) \\
&\qquad + |v^\varepsilon|^2 \big(- \eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp} \big) \Big] \Big\}
\end{aligned}
$$

$$
\begin{aligned}
= -\frac{1}{\mathcal{D}^\varepsilon} \Big\{ & \delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{\mathrm{s}} \big(- (v^\varepsilon)^2 (\overline{v^\varepsilon})^2 + (|v^\varepsilon|^2)^2 \big) \\
&+ \delta A^\varepsilon_k \delta A^\varepsilon_p \Big[- 2 v^k_\varepsilon \big(2|v^\varepsilon|^2 \overline{v^p_\varepsilon} - (\overline{v^\varepsilon})^2 v^p_\varepsilon \big) + (v^\varepsilon)^2 \big(2\overline{v^k_\varepsilon v^p_\varepsilon} - (\overline{v^\varepsilon})^2 \eta^{kp} \big) + (|v^\varepsilon|^2)^2 \eta^{kp} \Big] \\
&+ \delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq} \Big[- 4 v^k_\varepsilon \Big(4\overline{v^l_\varepsilon}\big(- v^p_\varepsilon \overline{v^q_\varepsilon} + 2 v^q_\varepsilon \overline{v^p_\varepsilon} \big) - 4|v^\varepsilon|^2 \big(- \eta^{lp} \overline{v^q_\varepsilon} + \eta^{lq} \overline{v^p_\varepsilon} \big) \\
&\qquad + 2(\overline{v^\varepsilon})^2 \big(- 2\eta^{lp} v^q_\varepsilon + \eta^{lq} v^p_\varepsilon \big) \Big) \\
&\quad + 4 v^l_\varepsilon \Big(4\overline{v^k_\varepsilon} v^q_\varepsilon \overline{v^p_\varepsilon} - 4|v^\varepsilon|^2 \big(- \eta^{kp} \overline{v^q_\varepsilon} + \eta^{kq} \overline{v^p_\varepsilon} \big) - 2(\overline{v^\varepsilon})^2 \eta^{kp} v^q_\varepsilon \Big) \\
&\quad - 4 (v^\varepsilon)^2 \Big(2\overline{v^k_\varepsilon}\big(- \eta^{lp} \overline{v^q_\varepsilon} + \eta^{lq} \overline{v^p_\varepsilon} \big) - 2\overline{v^l_\varepsilon}\big(- \eta^{kp} \overline{v^q_\varepsilon} + \eta^{kq} \overline{v^p_\varepsilon} \big) \\
&\qquad + (\overline{v^\varepsilon})^2 \big(- \eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp} \big) \Big) \\
&\qquad + 4(|v^\varepsilon|^2)^2 \big(- \eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp} \big) \Big] \Big\}
\end{aligned}
$$

$$
= -\frac{1}{\mathcal{D}^\varepsilon} \Big\{ \delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{\mathrm{s}} \big(- (v^\varepsilon)^2 (\overline{v^\varepsilon})^2 + (|v^\varepsilon|^2)^2 \big)
$$

$$
\begin{aligned}
&+ \delta A^\varepsilon_k \delta A^\varepsilon_p \Big[-4|v^\varepsilon|^2 v^k_\varepsilon \overline{v^p_\varepsilon} + 2\big((\overline{v^\varepsilon})^2 v^k_\varepsilon v^p_\varepsilon + (v^\varepsilon)^2 \overline{v^k_\varepsilon v^p_\varepsilon}\big) + \big((|v^\varepsilon|^2)^2 - (v^\varepsilon)^2(\overline{v^\varepsilon})^2\big)\eta^{kp}\Big] \\
&+ \delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq} \Big[16\Big(v^k_\varepsilon \overline{v^l_\varepsilon}\big(v^p_\varepsilon \overline{v^q_\varepsilon} - \overline{v^p_\varepsilon} v^q_\varepsilon\big) + \big(\overline{v^k_\varepsilon} v^l_\varepsilon - v^k_\varepsilon \overline{v^l_\varepsilon}\big)\overline{v^p_\varepsilon} v^q_\varepsilon \Big) \\
&\qquad + 8(\overline{v^\varepsilon})^2 \Big(v^k_\varepsilon\big(\eta^{lp} v^q_\varepsilon - \eta^{lq} v^p_\varepsilon\big) + \big(v^k_\varepsilon \eta^{lp} - v^l_\varepsilon \eta^{kp}\big) v^q_\varepsilon \Big) \\
&\qquad + 8\big(2|v^\varepsilon|^2 v^k_\varepsilon - (v^\varepsilon)^2 \overline{v^k_\varepsilon}\big)\big(-\eta^{lp}\overline{v^q_\varepsilon} + \eta^{lq}\overline{v^p_\varepsilon}\big) \\
&\qquad - 8\big(2|v^\varepsilon|^2 v^l_\varepsilon - (v^\varepsilon)^2 \overline{v^l_\varepsilon}\big)\big(-\eta^{kp}\overline{v^q_\varepsilon} + \eta^{kq}\overline{v^p_\varepsilon}\big) \\
&\qquad + 4\big((|v^\varepsilon|^2)^2 - (v^\varepsilon)^2(\overline{v^\varepsilon})^2\big)\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big)\Big]\Big\}
\end{aligned} \tag{B.16d}
$$

Adding up all four contributions yields

$$
\begin{aligned}
&\operatorname{Tr}\left(F^\varepsilon_\pm \delta A^\varepsilon F^\varepsilon_\mp \delta A^\varepsilon\right) = \\
&\overset{\text{(B.16)}}{=} \Big\{ \overset{(1.1)}{\cancel{\delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{\mathrm{s}}}} + \overset{(2.1)}{\cancel{\delta A^\varepsilon_k \delta A^\varepsilon_p \eta^{kp}}} + \overset{(3.1)}{\cancel{4\delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq}}}\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big) \Big\} \\
&\quad - \frac{1}{\mathcal{D}^\varepsilon} \Big\{ \overset{(1.2)}{\cancel{\delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{\mathrm{s}}}} \Big[(v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2 \Big] \\
&\qquad + \overset{(2.2)}{\cancel{\delta A^\varepsilon_k \delta A^\varepsilon_p}} \Big[2(v^k_\varepsilon \overline{s^\varepsilon} + \overline{v^k_\varepsilon} s^\varepsilon)(v^p_\varepsilon \overline{s^\varepsilon} + \overline{v^p_\varepsilon} s^\varepsilon) - \big((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2\big)\eta^{kp} \Big] \\
&\qquad + \overset{(3.2)}{\cancel{4\delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq}}} \Big[2(v^k_\varepsilon \overline{s^\varepsilon} + \overline{v^k_\varepsilon} s^\varepsilon)(v^p_\varepsilon \overline{s^\varepsilon} + \overline{v^p_\varepsilon} s^\varepsilon)\eta^{lq} + 2(v^l_\varepsilon \overline{s^\varepsilon} + \overline{v^l_\varepsilon} s^\varepsilon)(v^q_\varepsilon \overline{s^\varepsilon} + \overline{v^q_\varepsilon} s^\varepsilon)\eta^{kp} \\
&\qquad\qquad - 4(v^k_\varepsilon \overline{s^\varepsilon} + \overline{v^k_\varepsilon} s^\varepsilon)(v^q_\varepsilon \overline{s^\varepsilon} + \overline{v^q_\varepsilon} s^\varepsilon)\eta^{lp} \\
&\qquad\qquad + \big((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2\big)\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big) \Big] \Big\} \\
&\quad - \frac{1}{\mathcal{D}^\varepsilon} \Big\{ \overset{(4)}{\cancel{8\delta A^\varepsilon_k \delta A^\varepsilon_{pq}}} \Big[(v^k_\varepsilon \overline{s^\varepsilon} + \overline{v^k_\varepsilon} s^\varepsilon)\big(-v^p_\varepsilon \overline{v^q_\varepsilon} + v^q_\varepsilon \overline{v^p_\varepsilon}\big) - \big(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon s^\varepsilon}\big)\big(-\eta^{kp}\overline{v^q_\varepsilon} + \eta^{kq}\overline{v^p_\varepsilon}\big) \\
&\qquad\qquad + (B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon)\big(-\eta^{kp} v^q_\varepsilon + \eta^{kq} v^p_\varepsilon\big) - (v^p_\varepsilon \overline{s^\varepsilon} + \overline{v^p_\varepsilon} s^\varepsilon)\big(v^k_\varepsilon \overline{v^q_\varepsilon} - \overline{v^k_\varepsilon} v^q_\varepsilon\big) \\
&\qquad\qquad + (v^q_\varepsilon \overline{s^\varepsilon} + \overline{v^q_\varepsilon} s^\varepsilon)\big(v^k_\varepsilon \overline{v^p_\varepsilon} - \overline{v^k_\varepsilon} v^p_\varepsilon\big) \Big] \Big\} \\
&\quad - \frac{1}{\mathcal{D}^\varepsilon} \Big\{ \overset{(1.3)}{\cancel{\delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{\mathrm{s}}}} \Big[-(v^\varepsilon)^2(\overline{v^\varepsilon})^2 + (|v^\varepsilon|^2)^2 \Big] \\
&\qquad + \overset{(2.3)}{\cancel{\delta A^\varepsilon_k \delta A^\varepsilon_p}} \Big[-4|v^\varepsilon|^2 v^k_\varepsilon \overline{v^p_\varepsilon} + 2\big((\overline{v^\varepsilon})^2 v^k_\varepsilon v^p_\varepsilon + (v^\varepsilon)^2 \overline{v^k_\varepsilon v^p_\varepsilon}\big) + \big((|v^\varepsilon|^2)^2 - (v^\varepsilon)^2(\overline{v^\varepsilon})^2\big)\eta^{kp} \Big] \\
&\qquad + \overset{(3.3)}{\cancel{4\delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq}}} \Big[4\Big(v^k_\varepsilon \overline{v^l_\varepsilon}\big(v^p_\varepsilon \overline{v^q_\varepsilon} - \overline{v^p_\varepsilon} v^q_\varepsilon\big) + \big(\overline{v^k_\varepsilon} v^l_\varepsilon - v^k_\varepsilon \overline{v^l_\varepsilon}\big)\overline{v^p_\varepsilon} v^q_\varepsilon \Big) \\
&\qquad\qquad + 2(\overline{v^\varepsilon})^2 \Big(v^k_\varepsilon\big(\eta^{lp} v^q_\varepsilon - \eta^{lq} v^p_\varepsilon\big) + \big(v^k_\varepsilon \eta^{lp} - v^l_\varepsilon \eta^{kp}\big) v^q_\varepsilon \Big) \\
&\qquad\qquad + 2\big(2|v^\varepsilon|^2 v^k_\varepsilon - (v^\varepsilon)^2 \overline{v^k_\varepsilon}\big)\big(-\eta^{lp}\overline{v^q_\varepsilon} + \eta^{lq}\overline{v^p_\varepsilon}\big) \\
&\qquad\qquad - 2\big(2|v^\varepsilon|^2 v^l_\varepsilon - (v^\varepsilon)^2 \overline{v^l_\varepsilon}\big)\big(-\eta^{kp}\overline{v^q_\varepsilon} + \eta^{kq}\overline{v^p_\varepsilon}\big) \\
&\qquad\qquad + \big((|v^\varepsilon|^2)^2 - (v^\varepsilon)^2(\overline{v^\varepsilon})^2\big)\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big) \Big] \Big\}
\end{aligned}
$$

Sorting and combining terms results in

$$
\ldots = \delta A^\varepsilon_{\mathrm{s}} \delta A^\varepsilon_{\mathrm{s}} \Big\{ \overset{(1)}{\cancel{1}} - \frac{1}{\mathcal{D}^\varepsilon} \underbrace{\big(\big((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2\big) - (v^\varepsilon)^2(\overline{v^\varepsilon})^2 + (|v^\varepsilon|^2)^2\big)}_{= \cancelto{\text{cancels (1)}}{\mathcal{D}^\varepsilon}} \Big\}
$$

$$
\begin{aligned}
&+\delta A^\varepsilon_k \delta A^\varepsilon_p \Big\{ \cancelto{(2)}{\eta^{kp}} - \frac{1}{\mathcal{D}^\varepsilon}\Big[2(v^k_\varepsilon \overline{s^\varepsilon} + \overline{v^k_\varepsilon} s^\varepsilon)(v^p_\varepsilon \overline{s^\varepsilon} + \overline{v^p_\varepsilon} s^\varepsilon) - 2\big((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 \\
&\qquad + (\overline{v^\varepsilon})^2(s^\varepsilon)^2\big)\eta^{kp} - 4|v^\varepsilon|^2 v^k_\varepsilon \overline{v^p_\varepsilon} + 2\big((\overline{v^\varepsilon})^2 v^k_\varepsilon v^p_\varepsilon + (v^\varepsilon)^2 \overline{v^k_\varepsilon v^p_\varepsilon}\big) \\
&\qquad + \underbrace{\big((|v^\varepsilon|^2)^2 - (v^\varepsilon)^2(\overline{v^\varepsilon})^2 + ((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2)\big)}_{=\cancelto{\text{cancels (2)}}{\mathcal{D}^\varepsilon}} \eta^{kp}\Big]\Big\} \\[2ex]
&+ 4\delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}\Big\{ \cancelto{(3)}{\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big)} \\
&\qquad - \frac{1}{\mathcal{D}^\varepsilon}\Big[2(v^k_\varepsilon \overline{s^\varepsilon} + \overline{v^k_\varepsilon} s^\varepsilon)(v^p_\varepsilon \overline{s^\varepsilon} + \overline{v^p_\varepsilon} s^\varepsilon)\eta^{lq} + 2(v^l_\varepsilon \overline{s^\varepsilon} + \overline{v^l_\varepsilon} s^\varepsilon)(v^q_\varepsilon \overline{s^\varepsilon} + \overline{v^q_\varepsilon} s^\varepsilon)\eta^{kp} \\
&\qquad - 4(v^k_\varepsilon \overline{s^\varepsilon} + \overline{v^k_\varepsilon} s^\varepsilon)(v^q_\varepsilon \overline{s^\varepsilon} + \overline{v^q_\varepsilon} s^\varepsilon)\eta^{lp} \\
&\qquad + 4\Big(v^k_\varepsilon \overline{v^l_\varepsilon}\big(v^p_\varepsilon \overline{v^q_\varepsilon} - \overline{v^p_\varepsilon} v^q_\varepsilon\big) + \big(\overline{v^k_\varepsilon} v^l_\varepsilon - v^k_\varepsilon \overline{v^l_\varepsilon}\big)\overline{v^p_\varepsilon} v^q_\varepsilon\Big) \\
&\qquad + 2(\overline{v^\varepsilon})^2\Big(v^k_\varepsilon\big(\eta^{lp} v^q_\varepsilon - \eta^{lq} v^p_\varepsilon\big) + \big(v^k_\varepsilon \eta^{lp} - v^l_\varepsilon \eta^{kp}\big)v^q_\varepsilon\Big) \\
&\qquad + 2\big(2|v^\varepsilon|^2 v^k_\varepsilon - (v^\varepsilon)^2 \overline{v^k_\varepsilon}\big)\big(-\eta^{lp}\overline{v^q_\varepsilon} + \eta^{lq}\overline{v^p_\varepsilon}\big) \\
&\qquad - 2\big(2|v^\varepsilon|^2 v^l_\varepsilon - (v^\varepsilon)^2 \overline{v^l_\varepsilon}\big)\big(-\eta^{kp}\overline{v^q_\varepsilon} + \eta^{kq}\overline{v^p_\varepsilon}\big) \\
&\qquad + \underbrace{\big((|v^\varepsilon|^2)^2 - (v^\varepsilon)^2(\overline{v^\varepsilon})^2 + ((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2)\big)}_{=\cancelto{\text{cancels (3)}}{\mathcal{D}^\varepsilon}}\big(-\eta^{kp}\eta^{lq} + \eta^{kq}\eta^{lp}\big)\Big]\Big\} \\[2ex]
&- \frac{8}{\mathcal{D}^\varepsilon}\delta A^\varepsilon_k \delta A^\varepsilon_{pq}\Big\{ \cancelto{(4.1)}{(v^k_\varepsilon \overline{s^\varepsilon} + \overline{v^k_\varepsilon} s^\varepsilon)\big(-v^p_\varepsilon \overline{v^q_\varepsilon} + v^q_\varepsilon \overline{v^p_\varepsilon}\big)} - \cancelto{(4.2)}{\big(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon s^\varepsilon}\big)\big(-\eta^{kp}\overline{v^q_\varepsilon} + \eta^{kq}\overline{v^p_\varepsilon}\big)} \\
&\qquad + (B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon)\big(-\eta^{kp} v^q_\varepsilon + \eta^{kq} v^p_\varepsilon\big) - \cancel{(v^p_\varepsilon \overline{s^\varepsilon} + \overline{v^p_\varepsilon} s^\varepsilon)\big(v^k_\varepsilon \overline{v^q_\varepsilon} - \overline{v^k_\varepsilon} v^q_\varepsilon\big)} \\
&\qquad + \cancelto{(4.3)}{(v^q_\varepsilon \overline{s^\varepsilon} + \overline{v^q_\varepsilon} s^\varepsilon)\big(v^k_\varepsilon \overline{v^p_\varepsilon} - \overline{v^k_\varepsilon} v^p_\varepsilon\big)}\Big\} \\[2ex]
&= -\frac{2}{\mathcal{D}^\varepsilon}\delta A^\varepsilon_k \delta A^\varepsilon_p \Big\{ (v^k_\varepsilon \overline{s^\varepsilon} + \overline{v^k_\varepsilon} s^\varepsilon)(v^p_\varepsilon \overline{s^\varepsilon} + \overline{v^p_\varepsilon} s^\varepsilon) - \big((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2\big)\eta^{kp} \\
&\qquad + v^k_\varepsilon\big((\overline{v^\varepsilon})^2 v^p_\varepsilon - |v^\varepsilon|^2 \overline{v^p_\varepsilon}\big) + \underbrace{\big((v^\varepsilon)^2 \overline{v^k_\varepsilon} - |v^\varepsilon|^2 v^k_\varepsilon\big)\overline{v^p_\varepsilon}}_{k \leftrightarrow p}\Big\} \\[2ex]
&- \frac{8}{\mathcal{D}^\varepsilon}\delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}\Big\{ (v^k_\varepsilon \overline{s^\varepsilon} + \overline{v^k_\varepsilon} s^\varepsilon)\big((v^p_\varepsilon \overline{s^\varepsilon} + \overline{v^p_\varepsilon} s^\varepsilon)\eta^{lq} - (v^q_\varepsilon \overline{s^\varepsilon} + \overline{v^q_\varepsilon} s^\varepsilon)\eta^{lp}\big) \\
&\qquad + \Big((v^l_\varepsilon \overline{s^\varepsilon} + \overline{v^l_\varepsilon} s^\varepsilon)\eta^{kp} - (v^k_\varepsilon \overline{s^\varepsilon} + \overline{v^k_\varepsilon} s^\varepsilon)\eta^{lp}\Big)(v^q_\varepsilon \overline{s^\varepsilon} + \overline{v^q_\varepsilon} s^\varepsilon) \\
&\qquad + 2\big(v^k_\varepsilon \overline{v^l_\varepsilon}\big(v^p_\varepsilon \overline{v^q_\varepsilon} - \overline{v^p_\varepsilon} v^q_\varepsilon\big) + \underbrace{\big(\overline{v^k_\varepsilon} v^l_\varepsilon - v^k_\varepsilon \overline{v^l_\varepsilon}\big)\overline{v^p_\varepsilon} v^q_\varepsilon}_{(kl)\leftrightarrow(pq)}\big) \\
&\qquad + (\overline{v^\varepsilon})^2\Big(v^k_\varepsilon\big(\eta^{lp} v^q_\varepsilon - \eta^{lq} v^p_\varepsilon\big) + \big(v^k_\varepsilon \eta^{lp} - v^l_\varepsilon \eta^{kp}\big)v^q_\varepsilon\Big) \\
&\qquad + \big(|v^\varepsilon|^2 v^k_\varepsilon - (v^\varepsilon)^2 \overline{v^k_\varepsilon}\big)\big(\eta^{lq}\overline{v^p_\varepsilon} - \eta^{lp}\overline{v^q_\varepsilon}\big) \\
&\qquad - \big(|v^\varepsilon|^2 v^l_\varepsilon - (v^\varepsilon)^2 \overline{v^l_\varepsilon}\big)\big(\eta^{kq}\overline{v^p_\varepsilon} - \eta^{kp}\overline{v^q_\varepsilon}\big) \\
&\qquad + |v^\varepsilon|^2 v^k_\varepsilon\big(-\eta^{lp}\overline{v^q_\varepsilon} + \eta^{lq}\overline{v^p_\varepsilon}\big) - \underbrace{|v^\varepsilon|^2 v^l_\varepsilon\big(-\eta^{kp}\overline{v^q_\varepsilon} + \eta^{kq}\overline{v^p_\varepsilon}\big)}_{(kl)\leftrightarrow(pq)}\Big\} \\[2ex]
&- \frac{8}{\mathcal{D}^\varepsilon}\delta A^\varepsilon_k \delta A^\varepsilon_{pq}\Big[2(v^k_\varepsilon \overline{s^\varepsilon} + \overline{v^k_\varepsilon} s^\varepsilon)\big(\overline{v^p_\varepsilon} v^q_\varepsilon - v^p_\varepsilon \overline{v^q_\varepsilon}\big) - \big(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon s^\varepsilon}\big)\big(\eta^{kq}\overline{v^p_\varepsilon} - \eta^{kp}\overline{v^q_\varepsilon}\big) \\
&\qquad + (B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon)\big(\eta^{kq} v^p_\varepsilon - \eta^{kp} v^q_\varepsilon\big)\Big]\Big\} \qquad \text{(B.17)}
\end{aligned}
$$

In order to break this expression down into terms containing $v^\varepsilon_i, s^\varepsilon$ as well as the variations δv^ε_i and δs^ε, we rewrite the individual terms inside the curly brackets as real and imaginary parts. To this end, we interchange pairs of indices $(kl) \leftrightarrow (pq)$ in terms containing $\delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}$ as well as indices $k \leftrightarrow p$ in terms $\delta A^\varepsilon_k \delta A^\varepsilon_p$ and thus obtain

$$
\begin{aligned}
&\operatorname{Tr}\left(F^\varepsilon_\pm \delta A^\varepsilon F^\varepsilon_\mp \delta A^\varepsilon\right) = \\
&= -\frac{2}{\mathfrak{D}^\varepsilon}\delta A^\varepsilon_k \delta A^\varepsilon_p \Big\{ 4\operatorname{Re}\big[v^k_\varepsilon \overline{s^\varepsilon}\big]\operatorname{Re}\big[v^p_\varepsilon \overline{s^\varepsilon}\big] - \big((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2\big)\eta^{kp} \\
&\qquad\qquad + 2\operatorname{Re}\Big[v^k_\varepsilon\big((\overline{v^\varepsilon})^2 v^p_\varepsilon - |v^\varepsilon|^2\overline{v^p_\varepsilon}\big)\Big]\Big\} \\
&\quad - \frac{8}{\mathfrak{D}^\varepsilon}\delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}\Big\{ 4\operatorname{Re}\big[v^k_\varepsilon\overline{s^\varepsilon}\big]\Big(\operatorname{Re}\big[v^p_\varepsilon\overline{s^\varepsilon}\big]\eta^{lq} - \operatorname{Re}\big[v^q_\varepsilon\overline{s^\varepsilon}\big]\eta^{lp}\Big) \\
&\qquad + 4\Big(\operatorname{Re}\big[v^l_\varepsilon\overline{s^\varepsilon}\big]\eta^{kp} - \operatorname{Re}\big[v^k_\varepsilon\overline{s^\varepsilon}\big]\eta^{lp}\Big)\operatorname{Re}\big[v^q_\varepsilon\overline{s^\varepsilon}\big] - 8\operatorname{Im}\big[v^k_\varepsilon\overline{v^l_\varepsilon}\big]\operatorname{Im}\big[v^p_\varepsilon\overline{v^q_\varepsilon}\big] \\
&\qquad + (\overline{v^\varepsilon})^2 v^k_\varepsilon\big(\eta^{lp}v^q_\varepsilon - \eta^{lq}v^p_\varepsilon\big) + (\overline{v^\varepsilon})^2\big(v^k_\varepsilon\eta^{lp} - v^l_\varepsilon\eta^{kp}\big)v^q_\varepsilon \\
&\qquad + \big(|v^\varepsilon|^2 v^k_\varepsilon - (v^\varepsilon)^2\overline{v^k_\varepsilon}\big)\big(\eta^{lq}\overline{v^p_\varepsilon} - \eta^{lp}\overline{v^q_\varepsilon}\big) \\
&\qquad - \big(|v^\varepsilon|^2 v^l_\varepsilon - (v^\varepsilon)^2\overline{v^l_\varepsilon}\big)\big(\eta^{kq}\overline{v^p_\varepsilon} - \eta^{kp}\overline{v^q_\varepsilon}\big) \\
&\qquad + |v^\varepsilon|^2 v^k_\varepsilon\big(\eta^{lq}\overline{v^p_\varepsilon} - \eta^{lp}\overline{v^q_\varepsilon}\big) - |v^\varepsilon|^2\big(\eta^{pl}\overline{v^k_\varepsilon} - \eta^{pk}\overline{v^l_\varepsilon}\big)v^q_\varepsilon\Big\} \\
&\quad - \frac{8}{\mathfrak{D}^\varepsilon}\delta A^\varepsilon_k\delta A^\varepsilon_{pq}\Big\{ -8\mathrm{i}\operatorname{Re}\big[v^k_\varepsilon\overline{s^\varepsilon}\big]\operatorname{Im}\big[v^p_\varepsilon\overline{v^q_\varepsilon}\big] + 2\mathrm{i}\operatorname{Im}\Big[\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\big(\eta^{kq}v^p_\varepsilon - \eta^{kp}v^q_\varepsilon\big)\Big]\Big\}
\end{aligned}
$$

$$
\begin{aligned}
&= -\frac{2}{\mathfrak{D}^\varepsilon}\delta A^\varepsilon_k \delta A^\varepsilon_p \Big\{ 4\operatorname{Re}\big[v^k_\varepsilon \overline{s^\varepsilon}\big]\operatorname{Re}\big[v^p_\varepsilon \overline{s^\varepsilon}\big] - \big((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2\big)\eta^{kp} \\
&\qquad\qquad + 2\operatorname{Re}\Big[v^k_\varepsilon\big((\overline{v^\varepsilon})^2 v^p_\varepsilon - |v^\varepsilon|^2\overline{v^p_\varepsilon}\big)\Big]\Big\} \\
&\quad - \frac{8}{\mathfrak{D}^\varepsilon}\delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}\Big\{ \underbrace{4\operatorname{Re}\big[v^k_\varepsilon\overline{s^\varepsilon}\big]\Big(\operatorname{Re}\big[v^p_\varepsilon\overline{s^\varepsilon}\big]\eta^{lq} - \operatorname{Re}\big[v^q_\varepsilon\overline{s^\varepsilon}\big]\eta^{lp}\Big)}_{(kl)\leftrightarrow(pq)} \\
&\qquad + 4\Big(\operatorname{Re}\big[v^l_\varepsilon\overline{s^\varepsilon}\big]\eta^{kp} - \operatorname{Re}\big[v^k_\varepsilon\overline{s^\varepsilon}\big]\eta^{lp}\Big)\operatorname{Re}\big[v^q_\varepsilon\overline{s^\varepsilon}\big] - 8\operatorname{Im}\big[v^k_\varepsilon\overline{v^l_\varepsilon}\big]\operatorname{Im}\big[v^p_\varepsilon\overline{v^q_\varepsilon}\big] \\
&\qquad + v^k_\varepsilon\Big(\big(|v^\varepsilon|^2\overline{v^p_\varepsilon} - (\overline{v^\varepsilon})^2 v^p_\varepsilon\big)\eta^{lq} - \big(|v^\varepsilon|^2\overline{v^q_\varepsilon} - (\overline{v^\varepsilon})^2 v^q_\varepsilon\big)\eta^{lp}\Big) \\
&\qquad + \Big(-\overset{(1.1)}{\cancel{\big(|v^\varepsilon|^2\overline{v^k_\varepsilon} - (\overline{v^\varepsilon})^2 v^k_\varepsilon\big)\eta^{lp}}} + \overset{(2.1)}{\cancel{\big(|v^\varepsilon|^2\overline{v^l_\varepsilon} - (\overline{v^\varepsilon})^2 v^l_\varepsilon\big)\eta^{kp}}}\Big)v^q_\varepsilon \\
&\qquad + \big(|v^\varepsilon|^2 v^k_\varepsilon - (v^\varepsilon)^2\overline{v^k_\varepsilon}\big)\Big(\underbrace{\eta^{lq}\overline{v^p_\varepsilon}}_{(kl)\leftrightarrow(pq)} - \overset{(1.2)}{\cancel{\eta^{lp}\overline{v^q_\varepsilon}}}\Big) \\
&\qquad - \big(|v^\varepsilon|^2 v^l_\varepsilon - (v^\varepsilon)^2\overline{v^l_\varepsilon}\big)\Big(\underbrace{\eta^{kq}\overline{v^p_\varepsilon}}_{(kl)\leftrightarrow(pq)} - \overset{(2.2)}{\cancel{\eta^{kp}\overline{v^q_\varepsilon}}}\Big)\Big\} \\
&\quad - \frac{8}{\mathfrak{D}^\varepsilon}\delta A^\varepsilon_k\delta A^\varepsilon_{pq}\Big\{ -8\mathrm{i}\operatorname{Re}\big[v^k_\varepsilon\overline{s^\varepsilon}\big]\operatorname{Im}\big[v^p_\varepsilon\overline{v^q_\varepsilon}\big] + 2\mathrm{i}\operatorname{Im}\Big[\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\big(\eta^{kq}v^p_\varepsilon - \eta^{kp}v^q_\varepsilon\big)\Big]\Big\}
\end{aligned}
$$

$$
\begin{aligned}
&= -\frac{2}{\mathfrak{D}^\varepsilon}\delta A^\varepsilon_k \delta A^\varepsilon_p \Big\{ 4\operatorname{Re}\big[v^k_\varepsilon \overline{s^\varepsilon}\big]\operatorname{Re}\big[v^p_\varepsilon \overline{s^\varepsilon}\big] - \big((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2\big)\eta^{kp} \\
&\qquad\qquad + 2\operatorname{Re}\Big[v^k_\varepsilon\big((\overline{v^\varepsilon})^2 v^p_\varepsilon - |v^\varepsilon|^2\overline{v^p_\varepsilon}\big)\Big]\Big\}
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{8}{\mathcal{D}^\varepsilon} \delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq} \Big\{ 4 \operatorname{Re}\big[v^p_\varepsilon \overline{s^\varepsilon}\big] \Big(\operatorname{Re}\big[v^k_\varepsilon \overline{s^\varepsilon}\big] \eta^{ql} - \operatorname{Re}\big[v^l_\varepsilon \overline{s^\varepsilon}\big] \eta^{qk} \Big) \\
&\qquad + 4 \Big(\operatorname{Re}\big[v^l_\varepsilon \overline{s^\varepsilon}\big] \eta^{kp} - \operatorname{Re}\big[v^k_\varepsilon \overline{s^\varepsilon}\big] \eta^{lp} \Big) \operatorname{Re}\big[v^q_\varepsilon \overline{s^\varepsilon}\big] - 8 \operatorname{Im}\big[v^k_\varepsilon \overline{v^l_\varepsilon}\big] \operatorname{Im}\big[v^p_\varepsilon \overline{v^q_\varepsilon}\big] \\
&\qquad + v^k_\varepsilon \Big(\big(|v^\varepsilon|^2 \overline{v^p_\varepsilon} - (\overline{v^\varepsilon})^2 v^p_\varepsilon\big) \eta^{lq} - \big(|v^\varepsilon|^2 \overline{v^q_\varepsilon} - (\overline{v^\varepsilon})^2 v^q_\varepsilon\big) \eta^{lp} \Big) \\
&\qquad - 2 \operatorname{Re}\Big[\big(|v^\varepsilon|^2 \overline{v^k_\varepsilon} - (\overline{v^\varepsilon})^2 v^k_\varepsilon\big) \eta^{lp} v^q_\varepsilon \Big] + 2 \operatorname{Re}\Big[\big(|v^\varepsilon|^2 \overline{v^l_\varepsilon} - (\overline{v^\varepsilon})^2 v^l_\varepsilon\big) \eta^{kp} v^q_\varepsilon \Big] \\
&\qquad + \big(|v^\varepsilon|^2 v^p_\varepsilon - (v^\varepsilon)^2 \overline{v^p_\varepsilon}\big) \eta^{ql} \overline{v^k_\varepsilon} - \big(|v^\varepsilon|^2 v^q_\varepsilon - (v^\varepsilon)^2 \overline{v^q_\varepsilon}\big) \eta^{pl} \overline{v^k_\varepsilon} \Big\} \\
&- \frac{8}{\mathcal{D}^\varepsilon} \delta A^\varepsilon_k \delta A^\varepsilon_{pq} \Big\{ - 8\mathrm{i} \operatorname{Re}\big[v^k_\varepsilon \overline{s^\varepsilon}\big] \operatorname{Im}\big[v^p_\varepsilon \overline{v^q_\varepsilon}\big] + 2\mathrm{i} \operatorname{Im}\Big[\big(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big) \big(\eta^{kq} v^p_\varepsilon - \eta^{kp} v^q_\varepsilon\big) \Big] \Big\}
\end{aligned}
$$

$$
\begin{aligned}
= &- \frac{2}{\mathcal{D}^\varepsilon} \delta A^\varepsilon_k \delta A^\varepsilon_p \Big\{ 4 \operatorname{Re}\big[v^k_\varepsilon \overline{s^\varepsilon}\big] \operatorname{Re}\big[v^p_\varepsilon \overline{s^\varepsilon}\big] - ((v^\varepsilon)^2 (\overline{s^\varepsilon})^2 + 2 |v^\varepsilon|^2 |s^\varepsilon|^2 + (\overline{v^\varepsilon})^2 (s^\varepsilon)^2) \eta^{kp} \\
&\qquad + 2 \operatorname{Re}\Big[v^k_\varepsilon \big((\overline{v^\varepsilon})^2 v^p_\varepsilon - |v^\varepsilon|^2 \overline{v^p_\varepsilon} \big) \Big] \Big\} \\
&- \frac{8}{\mathcal{D}^\varepsilon} \delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq} \Big\{ 4 \Big(\operatorname{Re}\big[v^k_\varepsilon \overline{s^\varepsilon}\big] \eta^{lq} - \operatorname{Re}\big[v^l_\varepsilon \overline{s^\varepsilon}\big] \eta^{kq} \Big) \operatorname{Re}\big[v^p_\varepsilon \overline{s^\varepsilon}\big] \\
&\qquad - 4 \Big(\operatorname{Re}\big[v^k_\varepsilon \overline{s^\varepsilon}\big] \eta^{lp} - \operatorname{Re}\big[v^l_\varepsilon \overline{s^\varepsilon}\big] \eta^{kp} \Big) \operatorname{Re}\big[v^\varepsilon_q \overline{s^\varepsilon}\big] \\
&\qquad - 8 \operatorname{Im}\big[v^k_\varepsilon \overline{v^l_\varepsilon}\big] \operatorname{Im}\big[v^p_\varepsilon \overline{v^q_\varepsilon}\big] + 2 \operatorname{Re}\Big[v^k_\varepsilon \big(|v^\varepsilon|^2 \overline{v^p_\varepsilon} - (\overline{v^\varepsilon})^2 v^p_\varepsilon\big) \eta^{lq} \Big] \\
&\qquad \underbrace{- 2 \operatorname{Re}\Big[v^k_\varepsilon \big(|v^\varepsilon|^2 \overline{v^q_\varepsilon} - (\overline{v^\varepsilon})^2 v^q_\varepsilon\big) \eta^{lp} \Big]}_{(kl) \leftrightarrow (pq)} - 2 \operatorname{Re}\Big[\big(|v^\varepsilon|^2 \overline{v^k_\varepsilon} - (\overline{v^\varepsilon})^2 v^k_\varepsilon\big) \eta^{lp} v^q_\varepsilon \Big] \\
&\qquad + 2 \operatorname{Re}\Big[\big(|v^\varepsilon|^2 \overline{v^l_\varepsilon} - (\overline{v^\varepsilon})^2 v^l_\varepsilon\big) \eta^{kp} v^q_\varepsilon \Big] \Big\} \\
&- \frac{8}{\mathcal{D}^\varepsilon} \delta A^\varepsilon_k \delta A^\varepsilon_{pq} \Big\{ - 8\mathrm{i} \operatorname{Re}\big[v^k_\varepsilon \overline{s^\varepsilon}\big] \operatorname{Im}\big[v^p_\varepsilon \overline{v^q_\varepsilon}\big] + 2\mathrm{i} \operatorname{Im}\Big[\big(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big) \big(\eta^{kq} v^p_\varepsilon - \eta^{kp} v^q_\varepsilon\big) \Big] \Big\}
\end{aligned}
$$

To proceed, we group terms according to the type of η's in the second term which yields

$$
\begin{aligned}
&\operatorname{Tr}\big(F^\varepsilon_\pm \delta A^\varepsilon F^\varepsilon_\mp \delta A^\varepsilon\big) = \\
&= - \frac{2}{\mathcal{D}^\varepsilon} \delta A^\varepsilon_k \delta A^\varepsilon_p \Big\{ 4 \operatorname{Re}\big[v^k_\varepsilon \overline{s^\varepsilon}\big] \operatorname{Re}\big[v^p_\varepsilon \overline{s^\varepsilon}\big] - ((v^\varepsilon)^2 (\overline{s^\varepsilon})^2 + 2 |v^\varepsilon|^2 |s^\varepsilon|^2 + (\overline{v^\varepsilon})^2 (s^\varepsilon)^2) \eta^{kp} \\
&\qquad + 2 \operatorname{Re}\Big[v^k_\varepsilon \big((\overline{v^\varepsilon})^2 v^p_\varepsilon - |v^\varepsilon|^2 \overline{v^p_\varepsilon} \big) \Big] \Big\} \\
&\quad - \frac{8}{\mathcal{D}^\varepsilon} \delta A^\varepsilon_{kl} \delta A^\varepsilon_{pq} \Big\{ \eta^{lq} \Big(4 \operatorname{Re}\big[v^k_\varepsilon \overline{s^\varepsilon}\big] \operatorname{Re}\big[v^p_\varepsilon \overline{s^\varepsilon}\big] + 2 \operatorname{Re}\Big[v^k_\varepsilon \big(|v^\varepsilon|^2 \overline{v^p_\varepsilon} - (\overline{v^\varepsilon})^2 v^p_\varepsilon\big) \Big] \Big) \\
&\qquad - \eta^{kq} \Big(4 \operatorname{Re}\big[v^l_\varepsilon \overline{s^\varepsilon}\big] \operatorname{Re}\big[v^p_\varepsilon \overline{s^\varepsilon}\big] + 2 \operatorname{Re}\Big[v^p_\varepsilon \big(|v^\varepsilon|^2 \overline{v^l_\varepsilon} - (\overline{v^\varepsilon})^2 v^l_\varepsilon\big) \Big] \Big) \\
&\qquad - \eta^{lp} \Big(4 \operatorname{Re}\big[v^k_\varepsilon \overline{s^\varepsilon}\big] \operatorname{Re}\big[v^q_\varepsilon \overline{s^\varepsilon}\big] + 2 \operatorname{Re}\Big[\big(|v^\varepsilon|^2 \overline{v^k_\varepsilon} - (\overline{v^\varepsilon})^2 v^k_\varepsilon\big) v^q_\varepsilon \Big] \Big) \\
&\qquad + \eta^{kp} \Big(4 \operatorname{Re}\big[v^l_\varepsilon \overline{s^\varepsilon}\big] \operatorname{Re}\big[v^q_\varepsilon \overline{s^\varepsilon}\big] + 2 \operatorname{Re}\Big[\big(|v^\varepsilon|^2 \overline{v^l_\varepsilon} - (\overline{v^\varepsilon})^2 v^l_\varepsilon\big) v^q_\varepsilon \Big] \Big) \\
&\qquad - 8 \operatorname{Im}\big[v^k_\varepsilon \overline{v^l_\varepsilon}\big] \operatorname{Im}\big[v^p_\varepsilon \overline{v^q_\varepsilon}\big] \Big\} \\
&\quad - \frac{8}{\mathcal{D}^\varepsilon} \delta A^\varepsilon_k \delta A^\varepsilon_{pq} \Big\{ - 8\mathrm{i} \operatorname{Re}\big[v^k_\varepsilon \overline{s^\varepsilon}\big] \operatorname{Im}\big[v^p_\varepsilon \overline{v^q_\varepsilon}\big] + 2\mathrm{i} \operatorname{Im}\Big[\big(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big) \big(\eta^{kq} v^p_\varepsilon - \eta^{kp} v^q_\varepsilon\big) \Big] \Big\}
\end{aligned}
$$

Rewriting products of real parts by using the relation $\mathrm{Re}(x)\,\mathrm{Re}(y) = \frac{1}{2}\,\mathrm{Re}\big(x(y+\bar{y})\big)$ as well as the definitions $B^\varepsilon \overset{(3.15)}{=} |v^\varepsilon|^2 + |s^\varepsilon|^2$ and $C^\varepsilon \overset{(3.15)}{=} (\overline{v^\varepsilon})^2 - (\overline{s^\varepsilon})^2$ turns the expression into the form

$$\begin{aligned}
\ldots = &-\frac{2}{\mathcal{D}^\varepsilon}\delta A^\varepsilon_k \delta A^\varepsilon_p \Big\{ 4\,\mathrm{Re}\left[v^k_\varepsilon \overline{s^\varepsilon}\right]\mathrm{Re}\left[v^p_\varepsilon \overline{s^\varepsilon}\right] - \left((v^\varepsilon)^2(\overline{s^\varepsilon})^2 + 2|v^\varepsilon|^2|s^\varepsilon|^2 + (\overline{v^\varepsilon})^2(s^\varepsilon)^2\right)\eta^{kp} \\
&\qquad + 2\,\mathrm{Re}\left[v^k_\varepsilon\left((\overline{v^\varepsilon})^2 v^p_\varepsilon - |v^\varepsilon|^2\overline{v^p_\varepsilon}\right)\right]\Big\} \\
&- \frac{16}{\mathcal{D}^\varepsilon}\delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}\Big\{\eta^{lq}\Big(B^\varepsilon\,\mathrm{Re}\left[v^k_\varepsilon\overline{v^p_\varepsilon}\right] - \mathrm{Re}\left[C^\varepsilon v^k_\varepsilon v^p_\varepsilon\right]\Big) - \eta^{kq}\Big(B^\varepsilon\,\mathrm{Re}\left[\overline{v^l_\varepsilon}v^p_\varepsilon\right] - \mathrm{Re}\left[C^\varepsilon v^l_\varepsilon v^p_\varepsilon\right]\Big) \\
&\qquad \underbrace{-\,\eta^{lp}\Big(B^\varepsilon\,\mathrm{Re}\left[\overline{v^k_\varepsilon}v^q_\varepsilon\right] - \mathrm{Re}\left[C^\varepsilon v^k_\varepsilon v^q_\varepsilon\right]\Big)}_{(kl)\leftrightarrow(pq)} + \eta^{kp}\Big(B^\varepsilon\,\mathrm{Re}\left[\overline{v^l_\varepsilon}v^q_\varepsilon\right] - \mathrm{Re}\left[C^\varepsilon v^l_\varepsilon v^q_\varepsilon\right]\Big) \\
&\qquad - 4\,\mathrm{Im}\left[v^k_\varepsilon\overline{v^l_\varepsilon}\right]\mathrm{Im}\left[v^p_\varepsilon\overline{v^q_\varepsilon}\right]\Big\} \\
&- \frac{8}{\mathcal{D}^\varepsilon}\delta A^\varepsilon_k\delta A^\varepsilon_{pq}\Big\{-8\mathrm{i}\,\mathrm{Re}\left[v^k_\varepsilon\overline{s^\varepsilon}\right]\mathrm{Im}\left[v^p_\varepsilon\overline{v^q_\varepsilon}\right] + 2\mathrm{i}\,\mathrm{Im}\Big[(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon)\big(\eta^{kq}v^p_\varepsilon - \eta^{kp}v^q_\varepsilon\big)\Big]\Big\}
\end{aligned}$$

Pulling the components of the variation of the regularized closed chain inside the curly brackets, we arrive at the following intermediate result

$$\begin{aligned}
&\mathrm{Tr}\left(F^\varepsilon_\pm \delta A^\varepsilon F^\varepsilon_\mp \delta A^\varepsilon\right) = \\
&= -\frac{2}{\mathcal{D}^\varepsilon}\Big\{4\Big(\underbrace{\delta A^\varepsilon_k\,\mathrm{Re}\left[v^k_\varepsilon\overline{s^\varepsilon}\right]}_{(\mathbf{1})}\Big)^2 - 2\,\mathrm{Re}\left[(v^\varepsilon)^2(\overline{s^\varepsilon})^2 + |v^\varepsilon|^2|s^\varepsilon|^2\right]\underbrace{\left(\delta A^\varepsilon_k\delta A^\varepsilon_p\eta^{kp}\right)}_{(\mathbf{2})} \\
&\qquad + \underbrace{2\,\delta A^\varepsilon_k\delta A^\varepsilon_p\,\mathrm{Re}\left[v^k_\varepsilon\left((\overline{v^\varepsilon})^2 v^p_\varepsilon - |v^\varepsilon|^2\overline{v^p_\varepsilon}\right)\right]}_{(\mathbf{3})}\Big\} \\
&\quad - \frac{16}{\mathcal{D}^\varepsilon}\Big\{\underbrace{\left(\delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}\eta^{lq}\right)}_{(\mathbf{4})}\mathrm{Re}\left[B^\varepsilon v^k_\varepsilon\overline{v^p_\varepsilon} - C^\varepsilon v^k_\varepsilon v^p_\varepsilon\right] - 2\underbrace{\left(\delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}\eta^{kq}\right)}_{(\mathbf{5})}\mathrm{Re}\left[B^\varepsilon\overline{v^l_\varepsilon}v^p_\varepsilon - C^\varepsilon v^l_\varepsilon v^p_\varepsilon\right] \\
&\qquad + \underbrace{\left(\delta A^\varepsilon_{kl}\delta A^\varepsilon_{pq}\eta^{kp}\right)}_{(\mathbf{6})}\mathrm{Re}\left[B^\varepsilon\overline{v^l_\varepsilon}v^q_\varepsilon - C^\varepsilon v^l_\varepsilon v^q_\varepsilon\right] - 4\Big(\underbrace{\delta A^\varepsilon_{kl}\,\mathrm{Im}\left[v^k_\varepsilon\overline{v^l_\varepsilon}\right]}_{(\mathbf{7})}\Big)^2\Big\} \\
&\quad - \frac{8}{\mathcal{D}^\varepsilon}\Big\{-8\mathrm{i}\underbrace{\left(\delta A^\varepsilon_k\,\mathrm{Re}\left[v^k_\varepsilon\overline{s^\varepsilon}\right]\right)}_{=(\mathbf{1})}\underbrace{\left(\delta A^\varepsilon_{pq}\,\mathrm{Im}\left[v^p_\varepsilon\overline{v^q_\varepsilon}\right]\right)}_{=(\mathbf{7})} \\
&\qquad + 2\mathrm{i}\,\mathrm{Im}\left[(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon)v^p_\varepsilon\right]\underbrace{\left(\delta A^\varepsilon_k\delta A^\varepsilon_{pq}\eta^{kq}\right)}_{(\mathbf{8})} \\
&\qquad - 2\mathrm{i}\,\mathrm{Im}\left[(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon)v^q_\varepsilon\right]\underbrace{\left(\delta A^\varepsilon_k\delta A^\varepsilon_{pq}\eta^{kp}\right)}_{(\mathbf{9})}\Big\}
\end{aligned} \tag{B.18}$$

(c) Insertion of explicit expressions for components of $\delta A^\varepsilon_\pm$

Having arrived at this point, we need to insert the explicit expressions for the components of the first variation of the regularized closed chain as derived in Lemma 3.3.6.

(i) Evaluating the individual terms in (B.18)

By evaluating all the terms, we get summands which, irrespective of complex-conjugations, take the form

$$(\eta^{ij}v^\varepsilon_i\delta v^\varepsilon_j)(\eta^{ij}v^\varepsilon_i\delta v^\varepsilon_j) \qquad (\eta^{ij}v^\varepsilon_i\delta v^\varepsilon_j)\delta s^\varepsilon \qquad \delta s^\varepsilon\delta s^\varepsilon \qquad (\eta^{ij}\delta v^\varepsilon_i\delta v^\varepsilon_j) \tag{B.19}$$

Due to the fact that we have to take the real part of $\mathrm{Tr}\left(F^\varepsilon_\pm\delta A^\varepsilon F^\varepsilon_\mp\delta A^\varepsilon\right)$ at the very end, terms involving three or four complex-conjugations can be converted into terms which only carry one or no complex-conjugation, respectively. Making use of the relation $\mathrm{Re}(x)\,\mathrm{Re}(y) = \frac{1}{2}\,\mathrm{Re}(xy + x\bar{y})$ yields

$$
\begin{aligned}
(\mathbf{1}) \;&=\; \delta A^\varepsilon_k \,\mathrm{Re}\left[v^k_\varepsilon \overline{s^\varepsilon}\right] \\
&\overset{(3.21a,ii)}{=} 2\,\mathrm{Re}\left[\overline{s^\varepsilon}\delta v^\varepsilon_k + \delta s^\varepsilon \overline{v^\varepsilon_k}\right] \mathrm{Re}\left[v^k_\varepsilon \overline{s^\varepsilon}\right] \\
&=\; \mathrm{Re}\Big[(\overline{s^\varepsilon})^2 (v^k_\varepsilon \delta v^\varepsilon_k) + |v^\varepsilon|^2 \overline{s^\varepsilon}\delta s^\varepsilon + |s^\varepsilon|^2 (\overline{v^k_\varepsilon}\delta v^\varepsilon_k) + (\overline{v^\varepsilon})^2 s^\varepsilon \delta s^\varepsilon\Big] \\
&=\; \mathrm{Re}\Big[(\overline{s^\varepsilon})^2 (v^k_\varepsilon \delta v^\varepsilon_k) + |s^\varepsilon|^2 (\overline{v^k_\varepsilon}\delta v^\varepsilon_k) + \big(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta s^\varepsilon\Big]
\end{aligned}
\tag{B.20a}
$$

$$
\begin{aligned}
(\mathbf{2}) \;&=\; \delta A^\varepsilon_k \delta A^\varepsilon_p \eta^{kp} \\
&\overset{(3.21a,ii)}{=} 4\,\mathrm{Re}\left[\overline{s^\varepsilon}\delta v^\varepsilon_k + \delta s^\varepsilon \overline{v^\varepsilon_k}\right] \mathrm{Re}\left[\overline{s^\varepsilon}\delta v^\varepsilon_p + \delta s^\varepsilon \overline{v^\varepsilon_p}\right]\eta^{kp} \\
&=\; 2\Big(\,\mathrm{Re}\left[\left(\overline{s^\varepsilon}\delta v^\varepsilon_k + \delta s^\varepsilon \overline{v^\varepsilon_k}\right)\left(\overline{s^\varepsilon}\delta v^\varepsilon_p + \delta s^\varepsilon \overline{v^\varepsilon_p}\right) + \left(\overline{s^\varepsilon}\delta v^\varepsilon_k + \delta s^\varepsilon \overline{v^\varepsilon_k}\right)\left(s^\varepsilon \delta\overline{v^\varepsilon_p} + \delta\overline{s^\varepsilon} v^\varepsilon_p\right)\right]\Big)\eta^{kp} \\
&=\; 2\Big(\,\mathrm{Re}\left[(\overline{s^\varepsilon})^2(\delta v^k_\varepsilon \delta v^\varepsilon_k) + \overline{s^\varepsilon}\delta s^\varepsilon(\overline{v^k_\varepsilon}\delta v^\varepsilon_k) + \overline{s^\varepsilon}\delta s^\varepsilon(\overline{v^k_\varepsilon}\delta v^\varepsilon_k) + (\overline{v^\varepsilon})^2(\delta s^\varepsilon)^2\right] \\
&\qquad + \mathrm{Re}\left[|s^\varepsilon|^2(\delta v^k_\varepsilon \delta\overline{v^\varepsilon_k}) + \overline{s^\varepsilon}\delta\overline{s^\varepsilon}(v^k_\varepsilon \delta v^\varepsilon_k) + s^\varepsilon \delta s^\varepsilon(\overline{v^k_\varepsilon}\delta\overline{v^\varepsilon_k}) + |v^\varepsilon|^2 \delta s^\varepsilon \delta\overline{s^\varepsilon}\right]\Big) \\
&=\; 2\,\mathrm{Re}\Big[(\overline{s^\varepsilon})^2(\delta v^k_\varepsilon \delta v^\varepsilon_k) + |s^\varepsilon|^2(\delta v^k_\varepsilon \delta\overline{v^\varepsilon_k}) + 2\overline{s^\varepsilon}(\overline{v^k_\varepsilon}\delta v^\varepsilon_k)\delta s^\varepsilon \\
&\qquad\quad + \left((\overline{v^\varepsilon})^2(\delta s^\varepsilon)^2 + |v^\varepsilon|^2 \delta s^\varepsilon \delta\overline{s^\varepsilon}\right) + 2\overline{s^\varepsilon}(v^k_\varepsilon \delta v^\varepsilon_k)\delta\overline{s^\varepsilon}\Big]
\end{aligned}
\tag{B.20b}
$$

$$
\begin{aligned}
(\mathbf{3}) \;&=\; \delta A^\varepsilon_k \delta A^\varepsilon_p \,\mathrm{Re}\Big[v^k_\varepsilon\big((\overline{v^\varepsilon})^2 v^p_\varepsilon - |v^\varepsilon|^2 \overline{v^p_\varepsilon}\big)\Big] \\
&\overset{(3.21a,ii)}{=} 4\,\mathrm{Re}\left[\overline{s^\varepsilon}\delta v^\varepsilon_k + \delta s^\varepsilon \overline{v^\varepsilon_k}\right] \mathrm{Re}\left[\overline{s^\varepsilon}\delta v^\varepsilon_p + \delta s^\varepsilon \overline{v^\varepsilon_p}\right] \mathrm{Re}\Big[v^k_\varepsilon\big((\overline{v^\varepsilon})^2 v^p_\varepsilon - |v^\varepsilon|^2 \overline{v^p_\varepsilon}\big)\Big] \\
&=\; 2\,\mathrm{Re}\left[\overline{s^\varepsilon}\delta v^\varepsilon_k + \delta s^\varepsilon \overline{v^\varepsilon_k}\right] \times \\
&\quad \times \Big(\,\mathrm{Re}\left[\overline{s^\varepsilon} v^k_\varepsilon\big((\overline{v^\varepsilon})^2(v^p_\varepsilon \delta v^\varepsilon_p) - |v^\varepsilon|^2(\overline{v^p_\varepsilon}\delta v^\varepsilon_p)\big) + \delta s^\varepsilon v^k_\varepsilon \cancelto{0}{\big((\overline{v^\varepsilon})^2|v^\varepsilon|^2 - |v^\varepsilon|^2(\overline{v^\varepsilon})^2\big)}\right] \\
&\qquad + \mathrm{Re}\left[\overline{s^\varepsilon}\overline{v^k_\varepsilon}\big((v^\varepsilon)^2(\overline{v^p_\varepsilon}\delta v^\varepsilon_p) - |v^\varepsilon|^2(v^p_\varepsilon \delta v^\varepsilon_p)\big) + \delta s^\varepsilon \overline{v^k_\varepsilon}\big((v^\varepsilon)^2(\overline{v^\varepsilon})^2 - (|v^\varepsilon|^2)^2\big)\right]\Big) \\
&=\; 2\,\mathrm{Re}\left[\overline{s^\varepsilon}\delta v^\varepsilon_k + \delta s^\varepsilon \overline{v^\varepsilon_k}\right] \times \\
&\quad \times \mathrm{Re}\Big[v^k_\varepsilon\big((\overline{v^\varepsilon})^2 \overline{s^\varepsilon}(v^p_\varepsilon \delta v^\varepsilon_p) - |v^\varepsilon|^2 \overline{s^\varepsilon}(\overline{v^p_\varepsilon}\delta v^\varepsilon_p)\big) \\
&\qquad\quad + \overline{v^k_\varepsilon}\big((v^\varepsilon)^2 \overline{s^\varepsilon}(\overline{v^p_\varepsilon}\delta v^\varepsilon_p) - |v^\varepsilon|^2 \overline{s^\varepsilon}(v^p_\varepsilon \delta v^\varepsilon_p) + (v^\varepsilon)^2(\overline{v^\varepsilon})^2 \delta s^\varepsilon - (|v^\varepsilon|^2)^2 \delta s^\varepsilon\big)\Big] \\
&=\; \mathrm{Re}\Big[\overline{s^\varepsilon}(v^k_\varepsilon \delta v^\varepsilon_k)\big((\overline{v^\varepsilon})^2 \overline{s^\varepsilon}(v^p_\varepsilon \delta v^\varepsilon_p) - \cancelto{(1)}{|v^\varepsilon|^2 \overline{s^\varepsilon}(\overline{v^p_\varepsilon}\delta v^\varepsilon_p)}\big) \\
&\qquad + \overline{s^\varepsilon}(\overline{v^k_\varepsilon}\delta v^\varepsilon_k)\big((v^\varepsilon)^2 \overline{s^\varepsilon}(\overline{v^p_\varepsilon}\delta v^\varepsilon_p) - \cancelto{=(1)}{|v^\varepsilon|^2 \overline{s^\varepsilon}(v^p_\varepsilon \delta v^\varepsilon_p)} + \cancelto{(2)}{(v^\varepsilon)^2(\overline{v^\varepsilon})^2 \delta s^\varepsilon} - \cancelto{(3)}{(|v^\varepsilon|^2)^2 \delta s^\varepsilon}\big) \\
&\qquad + \delta s^\varepsilon |v^\varepsilon|^2 \big(\cancelto{(4)}{(\overline{v^\varepsilon})^2 \overline{s^\varepsilon}(v^p_\varepsilon \delta v^\varepsilon_p)} - \cancelto{=(3)}{|v^\varepsilon|^2 \overline{s^\varepsilon}(\overline{v^p_\varepsilon}\delta v^\varepsilon_p)}\big) \\
&\qquad + \delta s^\varepsilon (\overline{v^\varepsilon})^2 \big(\cancelto{=(2)}{(v^\varepsilon)^2 \overline{s^\varepsilon}(\overline{v^p_\varepsilon}\delta v^\varepsilon_p)} - \cancelto{\text{cancels }(4)}{|v^\varepsilon|^2 \overline{s^\varepsilon}(v^p_\varepsilon \delta v^\varepsilon_p)} + (v^\varepsilon)^2(\overline{v^\varepsilon})^2 \delta s^\varepsilon - (|v^\varepsilon|^2)^2 \delta s^\varepsilon\big)\Big] \\
&\quad + \mathrm{Re}\Big[s^\varepsilon(v^k_\varepsilon \delta\overline{v^\varepsilon_k})\big((\overline{v^\varepsilon})^2 \overline{s^\varepsilon}(v^p_\varepsilon \delta v^\varepsilon_p) - |v^\varepsilon|^2 \overline{s^\varepsilon}(\overline{v^p_\varepsilon}\delta v^\varepsilon_p)\big) \\
&\qquad + s^\varepsilon(\overline{v^k_\varepsilon}\delta\overline{v^\varepsilon_k})\big((v^\varepsilon)^2 \overline{s^\varepsilon}(\overline{v^p_\varepsilon}\delta v^\varepsilon_p) - |v^\varepsilon|^2 \overline{s^\varepsilon}(v^p_\varepsilon \delta v^\varepsilon_p) + (v^\varepsilon)^2(\overline{v^\varepsilon})^2 \delta s^\varepsilon - (|v^\varepsilon|^2)^2 \delta s^\varepsilon\big) \\
&\qquad + \delta\overline{s^\varepsilon}(v^\varepsilon)^2 \big((\overline{v^\varepsilon})^2 \overline{s^\varepsilon}(v^p_\varepsilon \delta v^\varepsilon_p) - \cancelto{(5)}{|v^\varepsilon|^2 \overline{s^\varepsilon}(\overline{v^p_\varepsilon}\delta v^\varepsilon_p)}\big) \\
&\qquad + \delta\overline{s^\varepsilon}|v^\varepsilon|^2 \big(\cancelto{\text{cancels }(5)}{(v^\varepsilon)^2 \overline{s^\varepsilon}(\overline{v^p_\varepsilon}\delta v^\varepsilon_p)} - |v^\varepsilon|^2 \overline{s^\varepsilon}(v^p_\varepsilon \delta v^\varepsilon_p) + (v^\varepsilon)^2(\overline{v^\varepsilon})^2 \delta s^\varepsilon - (|v^\varepsilon|^2)^2 \delta s^\varepsilon\big)\Big]
\end{aligned}
$$

$$
\begin{aligned}
&= \operatorname{Re}\Big[(\overline{v^\varepsilon})^2(\overline{s^\varepsilon})^2(v_\varepsilon^p\delta v_p^\varepsilon)^2 - 2|v^\varepsilon|^2(\overline{s^\varepsilon})^2(v_\varepsilon^k\delta v_k^\varepsilon)(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)\\
&\quad + (v^\varepsilon)^2(\overline{s^\varepsilon})^2(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)^2 + 2\big((v^\varepsilon)^2(\overline{v^\varepsilon})^2\overline{s^\varepsilon} - (|v^\varepsilon|^2)^2\overline{s^\varepsilon}\big)(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)\delta s^\varepsilon\\
&\quad + (\overline{v^\varepsilon})^2\big((v^\varepsilon)^2(\overline{v^\varepsilon})^2 - (|v^\varepsilon|^2)^2\big)(\delta s^\varepsilon)^2 + (\overline{v^\varepsilon})^2|s^\varepsilon|^2(v_\varepsilon^p\delta v_p^\varepsilon)(v_\varepsilon^k\overline{\delta v_k^\varepsilon})\\
&\quad - |v^\varepsilon|^2|s^\varepsilon|^2(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)(v_\varepsilon^k\overline{\delta v_k^\varepsilon}) + (v^\varepsilon)^2|s^\varepsilon|^2(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)(\overline{v_\varepsilon^k}\overline{\delta v_k^\varepsilon})\\
&\quad - |v^\varepsilon|^2|s^\varepsilon|^2(v_\varepsilon^p\delta v_p^\varepsilon)(\overline{v_\varepsilon^k}\overline{\delta v_k^\varepsilon}) + \big((v^\varepsilon)^2(\overline{v^\varepsilon})^2 s^\varepsilon - (|v^\varepsilon|^2)^2 s^\varepsilon\big)(\overline{v_\varepsilon^k}\overline{\delta v_k^\varepsilon})\delta s^\varepsilon\\
&\quad + \big((v^\varepsilon)^2(\overline{v^\varepsilon})^2\overline{s^\varepsilon} - (|v^\varepsilon|^2)^2\overline{s^\varepsilon}\big)(v_\varepsilon^p\delta v_p^\varepsilon)\overline{\delta s^\varepsilon} + \big(|v^\varepsilon|^2(v^\varepsilon)^2(\overline{v^\varepsilon})^2 - (|v^\varepsilon|^2)^3\big)\delta s^\varepsilon\overline{\delta s^\varepsilon}\Big]\\[1ex]
&= \operatorname{Re}\Big[(\overline{v^\varepsilon})^2(\overline{s^\varepsilon})^2(v_\varepsilon^p\delta v_p^\varepsilon)^2 - 2|v^\varepsilon|^2(\overline{s^\varepsilon})^2(v_\varepsilon^k\delta v_k^\varepsilon)(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)\\
&\quad + (v^\varepsilon)^2(\overline{s^\varepsilon})^2(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)^2 + 2\big((v^\varepsilon)^2(\overline{v^\varepsilon})^2\overline{s^\varepsilon} - (|v^\varepsilon|^2)^2\overline{s^\varepsilon}\big)(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)\delta s^\varepsilon\\
&\quad + (\overline{v^\varepsilon})^2\big((v^\varepsilon)^2(\overline{v^\varepsilon})^2 - (|v^\varepsilon|^2)^2\big)(\delta s^\varepsilon)^2 + (\overline{v^\varepsilon})^2|s^\varepsilon|^2\cancelto{(1)}{(v_\varepsilon^p\delta v_p^\varepsilon)(v_\varepsilon^k\overline{\delta v_k^\varepsilon})}\\
&\quad - |v^\varepsilon|^2|s^\varepsilon|^2(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)(v_\varepsilon^k\overline{\delta v_k^\varepsilon}) + (\overline{v^\varepsilon})^2|s^\varepsilon|^2\cancelto{=(1)}{(v_\varepsilon^p\overline{\delta v_p^\varepsilon})(v_\varepsilon^k\delta v_k^\varepsilon)}\\
&\quad - |v^\varepsilon|^2|s^\varepsilon|^2(v_\varepsilon^p\delta v_p^\varepsilon)(\overline{v_\varepsilon^k}\overline{\delta v_k^\varepsilon}) + \big((\overline{v^\varepsilon})^2(v^\varepsilon)^2\overline{s^\varepsilon} - (|v^\varepsilon|^2)^2\overline{s^\varepsilon}\big)\cancelto{(2)}{(v_\varepsilon^k\delta v_k^\varepsilon)\overline{\delta s^\varepsilon}}\\
&\quad + \big((v^\varepsilon)^2(\overline{v^\varepsilon})^2\overline{s^\varepsilon} - (|v^\varepsilon|^2)^2\overline{s^\varepsilon}\big)\cancelto{=(2)}{(v_\varepsilon^p\delta v_p^\varepsilon)\overline{\delta s^\varepsilon}} + \big(|v^\varepsilon|^2(v^\varepsilon)^2(\overline{v^\varepsilon})^2 - (|v^\varepsilon|^2)^3\big)\delta s^\varepsilon\overline{\delta s^\varepsilon}\Big]\\[1ex]
&= \operatorname{Re}\Big[(\overline{v^\varepsilon})^2(\overline{s^\varepsilon})^2(v_\varepsilon^p\delta v_p^\varepsilon)^2 - 2|v^\varepsilon|^2(\overline{s^\varepsilon})^2(v_\varepsilon^k\delta v_k^\varepsilon)(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)\\
&\quad + 2(\overline{v^\varepsilon})^2|s^\varepsilon|^2(v_\varepsilon^p\delta v_p^\varepsilon)(v_\varepsilon^k\overline{\delta v_k^\varepsilon}) + (v^\varepsilon)^2(\overline{s^\varepsilon})^2(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)^2\\
&\quad - |v^\varepsilon|^2|s^\varepsilon|^2\big((\overline{v_\varepsilon^p}\delta v_p^\varepsilon)(v_\varepsilon^k\overline{\delta v_k^\varepsilon}) + (v_\varepsilon^p\delta v_p^\varepsilon)(\overline{v_\varepsilon^k}\overline{\delta v_k^\varepsilon})\big)\\
&\quad + 2\overline{s^\varepsilon}\big((v^\varepsilon)^2(\overline{v^\varepsilon})^2 - (|v^\varepsilon|^2)^2\big)\big((\overline{v_\varepsilon^k}\delta v_k^\varepsilon)\delta s^\varepsilon + (v_\varepsilon^k\delta v_k^\varepsilon)\overline{\delta s^\varepsilon}\big)\\
&\quad + \big((v^\varepsilon)^2(\overline{v^\varepsilon})^2 - (|v^\varepsilon|^2)^2\big)\big((\overline{v^\varepsilon})^2(\delta s^\varepsilon)^2 + |v^\varepsilon|^2\delta s^\varepsilon\overline{\delta s^\varepsilon}\big)\Big] \qquad \text{(B.20c)}
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{(4)} &= \delta A_{kl}^\varepsilon \delta A_{pq}^\varepsilon \eta^{lq}\\
&\overset{(3.21a.i)}{=} \frac{1}{4}\big[\delta v_k^\varepsilon\overline{v_l^\varepsilon} + v_k^\varepsilon\overline{\delta v_l^\varepsilon}\big]\big[\delta v_p^\varepsilon\overline{v_q^\varepsilon} + v_p^\varepsilon\overline{\delta v_q^\varepsilon}\big]\eta^{lq}\\
&= \frac{1}{4}\big[(\overline{v^\varepsilon})^2\delta v_k^\varepsilon\delta v_p^\varepsilon + (\eta^{lq}\overline{v_q^\varepsilon}\overline{\delta v_l^\varepsilon})\delta v_k^\varepsilon v_p^\varepsilon + (\eta^{lq}\overline{v_q^\varepsilon}\overline{\delta v_l^\varepsilon})v_k^\varepsilon\delta v_p^\varepsilon + (\eta^{lq}\overline{\delta v_q^\varepsilon}\overline{\delta v_l^\varepsilon})v_k^\varepsilon v_p^\varepsilon\big]\\
&= \frac{1}{4}\big[(\overline{v^\varepsilon})^2\delta v_k^\varepsilon\delta v_p^\varepsilon + (\overline{v_\varepsilon^l}\overline{\delta v_l^\varepsilon})(\delta v_k^\varepsilon v_p^\varepsilon + v_k^\varepsilon\delta v_p^\varepsilon) + (\overline{\delta v_\varepsilon^l}\overline{\delta v_l^\varepsilon})v_k^\varepsilon v_p^\varepsilon\big] \qquad \text{(B.20d)}
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{(5)} &= \delta A_{kl}^\varepsilon \delta A_{pq}^\varepsilon \eta^{kq}\\
&\overset{(3.21a.i)}{=} \frac{1}{4}\big[\delta v_k^\varepsilon\overline{v_l^\varepsilon} + v_k^\varepsilon\overline{\delta v_l^\varepsilon}\big]\big[\delta v_p^\varepsilon\overline{v_q^\varepsilon} + v_p^\varepsilon\overline{\delta v_q^\varepsilon}\big]\eta^{kq}\\
&= \frac{1}{4}\big[(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)\overline{v_l^\varepsilon}\delta v_p^\varepsilon + (\delta v_\varepsilon^k\overline{\delta v_k^\varepsilon})\overline{v_l^\varepsilon}v_p^\varepsilon + |v^\varepsilon|^2\overline{\delta v_l^\varepsilon}\delta v_p^\varepsilon + (v_\varepsilon^k\overline{\delta v_k^\varepsilon})\overline{\delta v_l^\varepsilon}v_p^\varepsilon\big] \qquad \text{(B.20e)}
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{(6)} &= \delta A_{kl}^\varepsilon \delta A_{pq}^\varepsilon \eta^{kp}\\
&\overset{(3.21a.i)}{=} \frac{1}{4}\big[\delta v_k^\varepsilon\overline{v_l^\varepsilon} + v_k^\varepsilon\overline{\delta v_l^\varepsilon}\big]\big[\delta v_p^\varepsilon\overline{v_q^\varepsilon} + v_p^\varepsilon\overline{\delta v_q^\varepsilon}\big]\eta^{kp}\\
&= \frac{1}{4}\big[(\eta^{kp}\delta v_k^\varepsilon\delta v_p^\varepsilon)\overline{v_l^\varepsilon}\overline{v_q^\varepsilon} + (v_\varepsilon^k\delta v_k^\varepsilon)\overline{v_l^\varepsilon}\overline{\delta v_q^\varepsilon} + (v_\varepsilon^k\delta v_k^\varepsilon)\overline{\delta v_l^\varepsilon}\overline{v_q^\varepsilon} + (v^\varepsilon)^2\overline{\delta v_l^\varepsilon}\overline{\delta v_q^\varepsilon}\big]\\
&= \frac{1}{4}\big[(\delta v_\varepsilon^k\delta v_k^\varepsilon)\overline{v_l^\varepsilon}\overline{v_q^\varepsilon} + (v_\varepsilon^k\delta v_k^\varepsilon)(\overline{v_l^\varepsilon}\overline{\delta v_q^\varepsilon} + \overline{\delta v_l^\varepsilon}\overline{v_q^\varepsilon}) + (v^\varepsilon)^2\overline{\delta v_l^\varepsilon}\overline{\delta v_q^\varepsilon}\big] \qquad \text{(B.20f)}
\end{aligned}
$$

$$
\begin{aligned}
(\mathbf{7}) &= \delta A^\varepsilon_{pq}\,\mathrm{Im}\left[v^p_\varepsilon \overline{v^q_\varepsilon}\right] \\
&\overset{(3.21a,i)}{=} \frac{1}{4\mathrm{i}}\left[\delta v^\varepsilon_p \overline{v^\varepsilon_q} + v^\varepsilon_p \delta\overline{v^\varepsilon_q}\right]\left[v^p_\varepsilon \overline{v^q_\varepsilon} - \overline{v^p_\varepsilon} v^\varepsilon_q\right] \\
&= \frac{1}{4\mathrm{i}}\left[(\overline{v^\varepsilon})^2 (v^p_\varepsilon \delta v^\varepsilon_p) - |v^\varepsilon|^2 (\overline{v^p_\varepsilon}\delta v^\varepsilon_p) + (v^\varepsilon)^2 (\overline{v^p_\varepsilon}\delta\overline{v^\varepsilon_p}) - |v^\varepsilon|^2 (v^p_\varepsilon \delta\overline{v^\varepsilon_p})\right] \\
&= \frac{1}{2\mathrm{i}}\,\mathrm{Re}\left[(\overline{v^\varepsilon})^2 (v^p_\varepsilon \delta v^\varepsilon_p) - |v^\varepsilon|^2 (\overline{v^p_\varepsilon}\delta v^\varepsilon_p)\right]
\end{aligned}
\tag{B.20g}
$$

$$
\begin{aligned}
(\mathbf{8}) &= \delta A^\varepsilon_k \delta A^\varepsilon_{pq} \eta^{kq} \\
&\overset{(3.21a,i)}{\underset{(3.21a,ii)}{=}} \mathrm{Re}\left[\overline{s^\varepsilon}\delta v^\varepsilon_k + \delta s^\varepsilon \overline{v^\varepsilon_k}\right]\left[\delta v^\varepsilon_p \overline{v^\varepsilon_q} + v^\varepsilon_p \delta\overline{v^\varepsilon_q}\right]\eta^{kq} \\
&= \frac{1}{2}\left[\overline{s^\varepsilon}\delta v^\varepsilon_k + s^\varepsilon \delta\overline{v^\varepsilon_k} + \delta s^\varepsilon \overline{v^\varepsilon_k} + \delta\overline{s^\varepsilon} v^\varepsilon_k\right]\left[\delta v^\varepsilon_p \overline{v^\varepsilon_q} + v^\varepsilon_p \delta\overline{v^\varepsilon_q}\right]\eta^{kq} \\
&= \frac{1}{2}\Big[\big(\overline{s^\varepsilon}(\overline{v^k_\varepsilon}\delta v^\varepsilon_k) + s^\varepsilon(\overline{v^k_\varepsilon}\delta\overline{v^\varepsilon_k}) + \delta s^\varepsilon (\overline{v^\varepsilon})^2 + \delta\overline{s^\varepsilon}|v^\varepsilon|^2\big)\delta v^\varepsilon_p \\
&\qquad + \big(\overline{s^\varepsilon}(\delta v^k_\varepsilon \delta\overline{v^\varepsilon_k}) + s^\varepsilon(\delta\overline{v^k_\varepsilon}\delta\overline{v^\varepsilon_k}) + \delta s^\varepsilon(\overline{v^k_\varepsilon}\delta\overline{v^\varepsilon_k}) + \delta\overline{s^\varepsilon}(v^k_\varepsilon \delta\overline{v^\varepsilon_k})\big) v^\varepsilon_p\Big]
\end{aligned}
\tag{B.20h}
$$

$$
\begin{aligned}
(\mathbf{9}) &= \delta A^\varepsilon_k \delta A^\varepsilon_{pq} \eta^{kp} \\
&\overset{(3.21a,i)}{\underset{(3.21a,ii)}{=}} \mathrm{Re}\left[\overline{s^\varepsilon}\delta v^\varepsilon_k + \delta s^\varepsilon \overline{v^\varepsilon_k}\right]\left[\delta v^\varepsilon_p \overline{v^\varepsilon_q} + v^\varepsilon_p \delta\overline{v^\varepsilon_q}\right]\eta^{kp} \\
&= \frac{1}{2}\left[\overline{s^\varepsilon}\delta v^\varepsilon_k + s^\varepsilon \delta\overline{v^\varepsilon_k} + \delta s^\varepsilon \overline{v^\varepsilon_k} + \delta\overline{s^\varepsilon} v^\varepsilon_k\right]\left[\delta v^\varepsilon_p \overline{v^\varepsilon_q} + v^\varepsilon_p \delta\overline{v^\varepsilon_q}\right]\eta^{kp} \\
&= \frac{1}{2}\Big[\big(\overline{s^\varepsilon}(\delta v^k_\varepsilon \delta v^\varepsilon_k) + s^\varepsilon(\delta\overline{v^k_\varepsilon}\delta v^\varepsilon_k) + \delta s^\varepsilon(\overline{v^k_\varepsilon}\delta v^\varepsilon_k) + \delta\overline{s^\varepsilon}(v^k_\varepsilon \delta v^\varepsilon_k)\big)\overline{v^\varepsilon_q} \\
&\qquad + \big(\overline{s^\varepsilon}(v^k_\varepsilon \delta v^\varepsilon_k) + s^\varepsilon(v^k_\varepsilon \delta\overline{v^\varepsilon_k}) + \delta s^\varepsilon |v^\varepsilon|^2 + \delta\overline{s^\varepsilon}(v^\varepsilon)^2\big)\delta\overline{v^\varepsilon_q}\Big]
\end{aligned}
\tag{B.20i}
$$

(ii) Putting together the results

Inserting the above results for the terms (**1**) – (**9**) into the intermediate result (B.18), we find

$$
\begin{aligned}
&\mathrm{Tr}\left(F^\varepsilon_\pm \delta A^\varepsilon F^\varepsilon_\mp \delta A^\varepsilon\right) = \\
&\overset{(B.18)}{\underset{(B.20)}{=}} -\frac{2}{\mathfrak{D}^\varepsilon}\Bigg\{4\Big(\mathrm{Re}\Big[(\overline{s^\varepsilon})^2 (v^k_\varepsilon \delta v^\varepsilon_k) + |s^\varepsilon|^2 (\overline{v^k_\varepsilon}\delta v^\varepsilon_k) + \big(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta s^\varepsilon\Big]\Big)^2 \\
&\qquad - 2\,\mathrm{Re}\left[(v^\varepsilon)^2 (\overline{s^\varepsilon})^2 + |v^\varepsilon|^2 |s^\varepsilon|^2\right]\times \\
&\qquad\quad \times 2\,\mathrm{Re}\Big[(\overline{s^\varepsilon})^2 (\delta v^k_\varepsilon \delta v^\varepsilon_k) + |s^\varepsilon|^2 (\delta v^k_\varepsilon \delta\overline{v^\varepsilon_k}) + 2\overline{s^\varepsilon}(\overline{v^k_\varepsilon}\delta v^\varepsilon_k)\delta s^\varepsilon \\
&\qquad\qquad + \big((\overline{v^\varepsilon})^2 (\delta s^\varepsilon)^2 + |v^\varepsilon|^2 \delta s^\varepsilon \delta\overline{s^\varepsilon}\big) + 2\overline{s^\varepsilon}(v^k_\varepsilon \delta v^\varepsilon_k)\delta\overline{s^\varepsilon}\Big] \\
&\qquad + 2\Big(\mathrm{Re}\Big[(\overline{v^\varepsilon})^2 (\overline{s^\varepsilon})^2 (v^p_\varepsilon \delta v^\varepsilon_p)^2 - 2|v^\varepsilon|^2 (\overline{s^\varepsilon})^2 (v^k_\varepsilon \delta v^\varepsilon_k)(\overline{v^p_\varepsilon}\delta v^\varepsilon_p) \\
&\qquad\qquad + 2(\overline{v^\varepsilon})^2 |s^\varepsilon|^2 (v^p_\varepsilon \delta v^\varepsilon_p)(v^k_\varepsilon \delta\overline{v^\varepsilon_k}) + (v^\varepsilon)^2 (\overline{s^\varepsilon})^2 (\overline{v^p_\varepsilon}\delta v^\varepsilon_p)^2 \\
&\qquad\qquad - |v^\varepsilon|^2 |s^\varepsilon|^2 \big((\overline{v^p_\varepsilon}\delta v^\varepsilon_p)(v^k_\varepsilon \delta\overline{v^\varepsilon_k}) + (v^p_\varepsilon \delta v^\varepsilon_p)(\overline{v^k_\varepsilon}\delta\overline{v^\varepsilon_k})\big) \\
&\qquad\qquad + 2\overline{s^\varepsilon}\big((v^\varepsilon)^2 (\overline{v^\varepsilon})^2 - (|v^\varepsilon|^2)^2\big)\big((\overline{v^k_\varepsilon}\delta v^\varepsilon_k)\delta s^\varepsilon + (v^k_\varepsilon \delta v^\varepsilon_k)\delta\overline{s^\varepsilon}\big) \\
&\qquad\qquad + \big((v^\varepsilon)^2 (\overline{v^\varepsilon})^2 - (|v^\varepsilon|^2)^2\big)\big((\overline{v^\varepsilon})^2 (\delta s^\varepsilon)^2 + |v^\varepsilon|^2 \delta s^\varepsilon \delta\overline{s^\varepsilon}\big)\Big]\Big)\Bigg\}
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{16}{\mathfrak{D}^\varepsilon}\Bigg\{\underbrace{\frac{1}{4}\left[(\overline{v^\varepsilon})^2 \delta v^\varepsilon_k \delta v^\varepsilon_p + (\overline{v^l_\varepsilon}\delta\overline{v^\varepsilon_l})(\delta v^\varepsilon_k v^\varepsilon_p + v^\varepsilon_k \delta v^\varepsilon_p) + (\delta\overline{v^l_\varepsilon}\delta\overline{v^\varepsilon_l}) v^\varepsilon_k v^\varepsilon_p\right]\mathrm{Re}\left[v^k_\varepsilon\big(B^\varepsilon \overline{v^p_\varepsilon} - C^\varepsilon v^p_\varepsilon\big)\right]}_{(1)} \\
&\qquad - 2\cdot\frac{1}{4}\left[(\overline{v^k_\varepsilon}\delta v^\varepsilon_k)\overline{v^\varepsilon_l}\delta v^\varepsilon_p + (\delta v^k_\varepsilon \delta\overline{v^\varepsilon_k})\overline{v^\varepsilon_l} v^\varepsilon_p + |v^\varepsilon|^2 \delta\overline{v^\varepsilon_l}\delta v^\varepsilon_p + (v^k_\varepsilon \delta\overline{v^\varepsilon_k})\delta\overline{v^\varepsilon_l} v^\varepsilon_p\right]\times \\
&\qquad\quad \times \mathrm{Re}\left[v^p_\varepsilon\big(B^\varepsilon \overline{v^l_\varepsilon} - C^\varepsilon v^l_\varepsilon\big)\right]
\end{aligned}
$$

$$+\frac{1}{4}\underbrace{\Big[(\delta v_\varepsilon^k \delta v_k^\varepsilon)\overline{v_l^\varepsilon}\,\overline{v_q^\varepsilon} + (v_\varepsilon^k \delta v_k^\varepsilon)(\overline{v_l^\varepsilon}\,\overline{\delta v_q^\varepsilon} + \overline{\delta v_l^\varepsilon}\,\overline{v_q^\varepsilon}) + (v^\varepsilon)^2\,\overline{\delta v_l^\varepsilon}\,\overline{\delta v_q^\varepsilon}\Big]\operatorname{Re}\big[v_\varepsilon^q\big(B^\varepsilon\overline{v_\varepsilon^l} - C^\varepsilon v_\varepsilon^l\big)\big]}_{\text{replace } (l,q)\to(p,k) \text{ and combine with (1)}}$$
$$-4\Big(\frac{1}{2\mathrm{i}}\operatorname{Re}\big[(\overline{v^\varepsilon})^2(v_\varepsilon^p\delta v_p^\varepsilon) - |v^\varepsilon|^2(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)\big]\Big)^2\Bigg\}$$

$$-\frac{8}{\mathcal{D}^\varepsilon}\Bigg\{-8\mathrm{i}\operatorname{Re}\Big[(\overline{s^\varepsilon})^2(v_\varepsilon^k\delta v_k^\varepsilon) + |s^\varepsilon|^2(\overline{v_\varepsilon^k}\delta v_k^\varepsilon) + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta s^\varepsilon\Big]\times$$
$$\times\frac{1}{2\mathrm{i}}\operatorname{Re}\Big[(\overline{v^\varepsilon})^2(v_\varepsilon^p\delta v_p^\varepsilon) - |v^\varepsilon|^2(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)\Big]$$
$$+2\mathrm{i}\operatorname{Im}\Big[(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon)v_\varepsilon^p\Big]\times$$
$$\times\frac{1}{2}\Big[\underbrace{\big(\overline{s^\varepsilon}(\overline{v_\varepsilon^k}\delta v_k^\varepsilon) + s^\varepsilon(\overline{v_\varepsilon^k}\,\overline{\delta v_k^\varepsilon}) + \delta s^\varepsilon(\overline{v^\varepsilon})^2 + \overline{\delta s^\varepsilon}|v^\varepsilon|^2\big)\delta v_p^\varepsilon}_{(2)}$$
$$+\underbrace{\big(\overline{s^\varepsilon}(\delta v_\varepsilon^k\overline{\delta v_k^\varepsilon}) + s^\varepsilon(\overline{\delta v_\varepsilon^k}\,\overline{\delta v_k^\varepsilon}) + \delta s^\varepsilon(\overline{v_\varepsilon^k}\,\overline{\delta v_k^\varepsilon}) + \overline{\delta s^\varepsilon}(v_\varepsilon^k\overline{\delta v_k^\varepsilon})\big)v_p^\varepsilon}_{(3)}\Big]$$

$$-2\mathrm{i}\underbrace{\operatorname{Im}\Big[(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon)v_\varepsilon^q\Big]}_{\text{replace } q\to p}\times$$
$$\times\frac{1}{2}\Big[\underbrace{\big(\overline{s^\varepsilon}(\delta v_\varepsilon^k\delta v_k^\varepsilon) + s^\varepsilon(\overline{\delta v_\varepsilon^k}\delta v_k^\varepsilon) + \delta s^\varepsilon(\overline{v_\varepsilon^k}\delta v_k^\varepsilon) + \overline{\delta s^\varepsilon}(v_\varepsilon^k\delta v_k^\varepsilon)\big)\overline{v_q^\varepsilon}}_{\text{replace } q\to p \text{ and combine with (3)}}$$
$$+\underbrace{\big(\overline{s^\varepsilon}(v_\varepsilon^k\delta v_k^\varepsilon) + s^\varepsilon(v_\varepsilon^k\overline{\delta v_k^\varepsilon}) + \delta s^\varepsilon|v^\varepsilon|^2 + \overline{\delta s^\varepsilon}(v^\varepsilon)^2\big)\overline{\delta v_q^\varepsilon}}_{\text{replace } q\to p \text{ and combine with (2)}}\Big]\Bigg\}$$

Combining terms yields

$$= -\frac{2}{\mathcal{D}^\varepsilon}\Bigg\{4\Big(\operatorname{Re}\Big[(\overline{s^\varepsilon})^2(v_\varepsilon^k\delta v_k^\varepsilon) + |s^\varepsilon|^2(\overline{v_\varepsilon^k}\delta v_k^\varepsilon) + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\delta s^\varepsilon\Big]\Big)^2$$
$$-4\operatorname{Re}\big[(v^\varepsilon)^2(\overline{s^\varepsilon})^2 + |v^\varepsilon|^2|s^\varepsilon|^2\big]\times$$
$$\times\operatorname{Re}\Big[(\overline{s^\varepsilon})^2(\delta v_\varepsilon^k\delta v_k^\varepsilon) + |s^\varepsilon|^2(\delta v_\varepsilon^k\overline{\delta v_k^\varepsilon}) + 2\overline{s^\varepsilon}(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)\delta s^\varepsilon$$
$$+\big((\overline{v^\varepsilon})^2(\delta s^\varepsilon)^2 + |v^\varepsilon|^2\delta s^\varepsilon\overline{\delta s^\varepsilon}\big) + 2\overline{s^\varepsilon}(v_\varepsilon^k\delta v_k^\varepsilon)\overline{\delta s^\varepsilon}\Big]$$
$$+2\operatorname{Re}\Big[(\overline{v^\varepsilon})^2(\overline{s^\varepsilon})^2(v_\varepsilon^p\delta v_p^\varepsilon)^2 - 2|v^\varepsilon|^2(\overline{s^\varepsilon})^2(v_\varepsilon^k\delta v_k^\varepsilon)(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)$$
$$+2(\overline{v^\varepsilon})^2|s^\varepsilon|^2(v_\varepsilon^p\delta v_p^\varepsilon)(v_\varepsilon^k\overline{\delta v_k^\varepsilon}) + (v^\varepsilon)^2(\overline{s^\varepsilon})^2(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)^2$$
$$-|v^\varepsilon|^2|s^\varepsilon|^2\big((\overline{v_\varepsilon^p}\delta v_p^\varepsilon)(v_\varepsilon^k\overline{\delta v_k^\varepsilon}) + (v_\varepsilon^p\delta v_p^\varepsilon)(\overline{v_\varepsilon^k}\,\overline{\delta v_k^\varepsilon})\big)$$
$$+2\overline{s^\varepsilon}\big((v^\varepsilon)^2(\overline{v^\varepsilon})^2 - (|v^\varepsilon|^2)^2\big)\big((\overline{v_\varepsilon^k}\delta v_k^\varepsilon)\delta s^\varepsilon + (v_\varepsilon^k\delta v_k^\varepsilon)\overline{\delta s^\varepsilon}\big)$$
$$+\big((v^\varepsilon)^2(\overline{v^\varepsilon})^2 - (|v^\varepsilon|^2)^2\big)\big((\overline{v^\varepsilon})^2(\delta s^\varepsilon)^2 + |v^\varepsilon|^2\delta s^\varepsilon\overline{\delta s^\varepsilon}\big)\Big]\Bigg\}$$

$$-\frac{16}{\mathcal{D}^\varepsilon}\Bigg\{\frac{1}{2}\operatorname{Re}\Big[(\overline{v^\varepsilon})^2\delta v_k^\varepsilon\delta v_p^\varepsilon + (\overline{v_\varepsilon^l}\,\overline{\delta v_l^\varepsilon})(\delta v_k^\varepsilon v_p^\varepsilon + v_k^\varepsilon\delta v_p^\varepsilon) + (\overline{\delta v_\varepsilon^l}\,\overline{\delta v_l^\varepsilon})v_k^\varepsilon v_p^\varepsilon\Big]\times$$
$$\times\operatorname{Re}\big[v_\varepsilon^k\big(B^\varepsilon\overline{v_\varepsilon^p} - C^\varepsilon v_\varepsilon^p\big)\big]$$
$$-\frac{1}{2}\Big[(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)\overline{v_l^\varepsilon}\delta v_p^\varepsilon + (\delta v_\varepsilon^k\overline{\delta v_k^\varepsilon})\overline{v_l^\varepsilon}v_p^\varepsilon + |v^\varepsilon|^2\overline{\delta v_l^\varepsilon}\delta v_p^\varepsilon + (v_\varepsilon^k\overline{\delta v_k^\varepsilon})\overline{\delta v_l^\varepsilon}v_p^\varepsilon\Big]\times$$
$$\times\operatorname{Re}\big[v_\varepsilon^p\big(B^\varepsilon\overline{v_\varepsilon^l} - C^\varepsilon v_\varepsilon^l\big)\big] + \Big(\operatorname{Re}\big[(\overline{v^\varepsilon})^2(v_\varepsilon^p\delta v_p^\varepsilon) - |v^\varepsilon|^2(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)\big]\Big)^2\Bigg\}$$

$$
\begin{aligned}
&-\frac{8}{\mathcal{D}^\varepsilon}\Bigg\{-4\,\mathrm{Re}\Big[(\overline{s^\varepsilon})^2(v_\varepsilon^k\delta v_k^\varepsilon)+|s^\varepsilon|^2(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)+\big(B^\varepsilon\overline{s^\varepsilon}+C^\varepsilon s^\varepsilon\big)\delta s^\varepsilon\Big]\times\\
&\qquad\times\mathrm{Re}\Big[(\overline{v^\varepsilon})^2(v_\varepsilon^p\delta v_p^\varepsilon)-|v^\varepsilon|^2(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)\Big]\\
&\quad-2\,\mathrm{Im}\Big[(B^\varepsilon\overline{s^\varepsilon}+C^\varepsilon s^\varepsilon)v_\varepsilon^p\Big]\times\\
&\qquad\times\mathrm{Im}\Big[\big(\overline{s^\varepsilon}(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)+s^\varepsilon(\overline{v_\varepsilon^k}\overline{\delta v_k^\varepsilon})+\delta s^\varepsilon(\overline{v^\varepsilon})^2+\overline{\delta s^\varepsilon}|v^\varepsilon|^2\big)\delta v_p^\varepsilon\\
&\qquad\qquad+\big(\overline{s^\varepsilon}(\delta v_\varepsilon^k\overline{\delta v_k^\varepsilon})+s^\varepsilon(\overline{\delta v_\varepsilon^k}\overline{\delta v_k^\varepsilon})+\delta s^\varepsilon(\overline{v_\varepsilon^k}\overline{\delta v_k^\varepsilon})+\overline{\delta s^\varepsilon}(v_\varepsilon^k\overline{\delta v_k^\varepsilon})\big)v_p^\varepsilon\Big]\Bigg\}
\end{aligned}
$$

Expanding products of two real or two imaginary parts by using the relations $\mathrm{Re}(x)\,\mathrm{Re}(y)=\frac{1}{2}\,\mathrm{Re}(xy+x\bar{y})$ and $\mathrm{Im}(x)\,\mathrm{Im}(y)=-\frac{1}{2}\,\mathrm{Re}(x(y-\bar{y}))$, respectively, and collecting terms with the curly brackets gives

$$
\begin{aligned}
\ldots=-\frac{2}{\mathcal{D}^\varepsilon}\Bigg\{&2\,\mathrm{Re}\Big[((\overline{s^\varepsilon})^2)^2\cancelto{(1.1)}{(v_\varepsilon^k\delta v_k^\varepsilon)^2}+|s^\varepsilon|^2(\overline{s^\varepsilon})^2\cancelto{(2.1)}{(v_\varepsilon^k\delta v_k^\varepsilon)(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)}\\
&+\big(B^\varepsilon\overline{s^\varepsilon}+C^\varepsilon s^\varepsilon\big)(\overline{s^\varepsilon})^2\cancelto{(3.1)}{(v_\varepsilon^k\delta v_k^\varepsilon)\delta s^\varepsilon}\\
&+(s^\varepsilon)^2(\overline{s^\varepsilon})^2\cancelto{(4.1)}{(v_\varepsilon^k\delta v_k^\varepsilon)(\overline{v_\varepsilon^k}\overline{\delta v_k^\varepsilon})}+|s^\varepsilon|^2(\overline{s^\varepsilon})^2\cancelto{(5.1)}{(v_\varepsilon^k\delta v_k^\varepsilon)(v_\varepsilon^k\overline{\delta v_k^\varepsilon})}\\
&+\big(B^\varepsilon s^\varepsilon+\overline{C^\varepsilon s^\varepsilon}\big)(\overline{s^\varepsilon})^2\cancelto{(6.1)}{(v_\varepsilon^k\delta v_k^\varepsilon)\overline{\delta s^\varepsilon}}\\
&+|s^\varepsilon|^2(\overline{s^\varepsilon})^2\cancelto{(2.2)}{(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)(v_\varepsilon^k\delta v_k^\varepsilon)}+(|s^\varepsilon|^2)^2\cancelto{(7.1)}{(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)^2}\\
&+\big(B^\varepsilon\overline{s^\varepsilon}+C^\varepsilon s^\varepsilon\big)|s^\varepsilon|^2\cancelto{(8.1)}{(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)\delta s^\varepsilon}\\
&+|s^\varepsilon|^2(s^\varepsilon)^2\cancelto{(5.2)}{(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)(\overline{v_\varepsilon^k}\overline{\delta v_k^\varepsilon})}+(|s^\varepsilon|^2)^2\cancelto{(9.1)}{(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)(v_\varepsilon^k\overline{\delta v_k^\varepsilon})}\\
&+\big(B^\varepsilon s^\varepsilon+\overline{C^\varepsilon s^\varepsilon}\big)|s^\varepsilon|^2\cancelto{(10.1)}{(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)\overline{\delta s^\varepsilon}}\\
&+\big(B^\varepsilon\overline{s^\varepsilon}+C^\varepsilon s^\varepsilon\big)(\overline{s^\varepsilon})^2\cancelto{(3.2)}{\delta s^\varepsilon(v_\varepsilon^k\delta v_k^\varepsilon)}+\big(B^\varepsilon\overline{s^\varepsilon}+C^\varepsilon s^\varepsilon\big)|s^\varepsilon|^2\cancelto{(8.2)}{(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)\delta s^\varepsilon}\\
&+\big(B^\varepsilon\overline{s^\varepsilon}+C^\varepsilon s^\varepsilon\big)^2\cancelto{(11.1)}{(\delta s^\varepsilon)^2}+\big(B^\varepsilon\overline{s^\varepsilon}+C^\varepsilon s^\varepsilon\big)(s^\varepsilon)^2\cancelto{(6.2)}{(\overline{v_\varepsilon^k}\overline{\delta v_k^\varepsilon})\delta s^\varepsilon}\\
&+\big(B^\varepsilon\overline{s^\varepsilon}+C^\varepsilon s^\varepsilon\big)|s^\varepsilon|^2\cancelto{(10.2)}{(v_\varepsilon^k\overline{\delta v_k^\varepsilon})\delta s^\varepsilon}+\big(B^\varepsilon s^\varepsilon+\overline{C^\varepsilon s^\varepsilon}\big)\big(B^\varepsilon\overline{s^\varepsilon}+C^\varepsilon s^\varepsilon\big)\cancelto{(12.1)}{\delta s^\varepsilon\,\overline{\delta s^\varepsilon}}\Big]\\[1em]
&-2\,\mathrm{Re}\Big[\big((v^\varepsilon)^2(\overline{s^\varepsilon})^2+(\overline{v^\varepsilon})^2(s^\varepsilon)^2+2|v^\varepsilon|^2|s^\varepsilon|^2\big)\times\\
&\quad\times\big((\overline{s^\varepsilon})^2\cancelto{(13.1)}{(\delta v_\varepsilon^k\overline{\delta v_k^\varepsilon})}+|s^\varepsilon|^2\cancelto{(14.1)}{(\overline{\delta v_\varepsilon^k}\overline{\delta v_k^\varepsilon})}+2\overline{s^\varepsilon}\cancelto{(8.3)}{(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)\delta s^\varepsilon}\\
&\qquad+(\overline{v^\varepsilon})^2\cancelto{(11.2)}{(\delta s^\varepsilon)^2}+|v^\varepsilon|^2\cancelto{(12.2)}{\delta s^\varepsilon\,\overline{\delta s^\varepsilon}}+2\overline{s^\varepsilon}\cancelto{(6.3)}{(v_\varepsilon^k\delta v_k^\varepsilon)\overline{\delta s^\varepsilon})}\Big]\\
&+2\,\mathrm{Re}\Big[(\overline{v^\varepsilon})^2(\overline{s^\varepsilon})^2\cancelto{(1.2)}{(v_\varepsilon^p\delta v_p^\varepsilon)^2}-2|v^\varepsilon|^2(\overline{s^\varepsilon})^2\cancelto{(2.3)}{(v_\varepsilon^k\delta v_k^\varepsilon)(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)}\\
&\quad+2(\overline{v^\varepsilon})^2|s^\varepsilon|^2\cancelto{(5.3)}{(v_\varepsilon^p\delta v_p^\varepsilon)(v_\varepsilon^k\overline{\delta v_k^\varepsilon})}+(v^\varepsilon)^2(\overline{s^\varepsilon})^2\cancelto{(7.2)}{(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)^2}\\
&\quad-|v^\varepsilon|^2|s^\varepsilon|^2\big(\cancelto{(9.2)}{(\overline{v_\varepsilon^p}\delta v_p^\varepsilon)(v_\varepsilon^k\overline{\delta v_k^\varepsilon})}+\cancelto{(4.2)}{(v_\varepsilon^p\delta v_p^\varepsilon)(\overline{v_\varepsilon^k}\overline{\delta v_k^\varepsilon})}\big)\\
&\quad+2\overline{s^\varepsilon}\big((v^\varepsilon)^2(\overline{v^\varepsilon})^2-(|v^\varepsilon|^2)^2\big)\big(\cancelto{(8.4)}{(\overline{v_\varepsilon^k}\delta v_k^\varepsilon)\delta s^\varepsilon}+\cancelto{(6.4)}{(v_\varepsilon^k\delta v_k^\varepsilon)\overline{\delta s^\varepsilon}}\big)\\
&\quad+(\overline{v^\varepsilon})^2\big((v^\varepsilon)^2(\overline{v^\varepsilon})^2-(|v^\varepsilon|^2)^2\big)\cancelto{(11.3)}{(\delta s^\varepsilon)^2}+|v^\varepsilon|^2\big((v^\varepsilon)^2(\overline{v^\varepsilon})^2-(|v^\varepsilon|^2)^2\big)\cancelto{(12.3)}{\delta s^\varepsilon\,\overline{\delta s^\varepsilon}}\Big]\Bigg\}
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{16}{\mathcal{D}^\varepsilon}\Bigg\{\frac{1}{2}B^\varepsilon \operatorname{Re}\Big[\cancelto{(15)}{(\overline{v^\varepsilon})^2(v^k_\varepsilon\delta v^\varepsilon_k)(\overline{v^p_\varepsilon\delta v^\varepsilon_p})} + (\overline{v^l_\varepsilon\delta v^\varepsilon_l})\big(\cancelto{(4.3)}{(v^k_\varepsilon\delta v^\varepsilon_k)}|v^\varepsilon|^2 + (v^\varepsilon)^2\cancelto{(5.4)}{(\overline{v^p_\varepsilon\delta v^\varepsilon_p})}\big) \\
&\qquad\qquad + \cancelto{(13.2)}{(\overline{\delta v^l_\varepsilon\delta v^\varepsilon_l})}(\overline{v^\varepsilon})^2|v^\varepsilon|^2\Big] \\
&\quad - \frac{1}{4}\operatorname{Re}\Big[C^\varepsilon\Big((\overline{v^\varepsilon})^2\cancelto{(1.3)}{(v^k_\varepsilon\delta v^\varepsilon_k)(v^p_\varepsilon\delta v^\varepsilon_p)} + 2\cancelto{(4.4)}{(\overline{v^l_\varepsilon\delta v^\varepsilon_l})(v^k_\varepsilon\delta v^\varepsilon_k)}(v^\varepsilon)^2 + \cancelto{(13.3)}{(\overline{\delta v^l_\varepsilon\delta v^\varepsilon_l})}(\overline{v^\varepsilon})^2(v^\varepsilon)^2\Big) \\
&\qquad + \overline{C^\varepsilon}\Big((\overline{v^\varepsilon})^2\cancelto{(7.3)}{(\overline{v^k_\varepsilon\delta v^\varepsilon_k})(\overline{v^p_\varepsilon\delta v^\varepsilon_p})} + 2\cancelto{(5.5)}{(\overline{v^l_\varepsilon\delta v^\varepsilon_l})(\overline{v^k_\varepsilon\delta v^\varepsilon_k})}|v^\varepsilon|^2 + \cancelto{(13.4)}{(\overline{\delta v^l_\varepsilon\delta v^\varepsilon_l})}(|v^\varepsilon|^2)^2\Big)\Big] \\
&\quad - \frac{1}{2}B^\varepsilon\Big(\operatorname{Re}\Big[\cancelto{\text{cancels (15)}}{(\overline{v^k_\varepsilon\delta v^\varepsilon_k})(\overline{v^\varepsilon})^2(v^p_\varepsilon\delta v^\varepsilon_p)}\Big] + \operatorname{Re}\Big[\cancelto{(7.4)}{(\overline{v^k_\varepsilon\delta v^\varepsilon_k})|v^\varepsilon|^2(\overline{v^p_\varepsilon\delta v^\varepsilon_p})}\Big]\Big) \\
&\quad - \frac{1}{4}B^\varepsilon\Big(\cancelto{(14.2)}{(\overline{\delta v^k_\varepsilon\delta v^\varepsilon_k})}(\overline{v^\varepsilon})^2(v^\varepsilon)^2 + |v^\varepsilon|^2\cancelto{(4.5)}{(\overline{v^k_\varepsilon\delta v^\varepsilon_k})(v^p_\varepsilon\delta v^\varepsilon_p)} \\
&\qquad + \cancelto{(14.3)}{(\overline{\delta v^k_\varepsilon\delta v^\varepsilon_k})}(|v^\varepsilon|^2)^2 + |v^\varepsilon|^2\cancelto{(9.3)}{(v^l_\varepsilon\delta v^\varepsilon_k)(\overline{v^p_\varepsilon\delta v^\varepsilon_p})}\Big) \\
&\quad + \frac{1}{2}\operatorname{Re}\Big[C^\varepsilon\Big(\cancelto{(2.4)}{(\overline{v^k_\varepsilon\delta v^\varepsilon_k})|v^\varepsilon|^2(v^p_\varepsilon\delta v^\varepsilon_p)} + \cancelto{(14.4)}{(\overline{\delta v^k_\varepsilon\delta v^\varepsilon_k})}|v^\varepsilon|^2(v^\varepsilon)^2 \\
&\qquad + |v^\varepsilon|^2\cancelto{(5.6)}{(\overline{v^l_\varepsilon\delta v^\varepsilon_l})(\overline{v^p_\varepsilon}\delta v^\varepsilon_p)} + \cancelto{(7.5)}{(v^k_\varepsilon\delta v^\varepsilon_k)(\overline{v^l_\varepsilon\delta v^\varepsilon_l})}(v^\varepsilon)^2\Big)\Big] \\
&\quad + \frac{1}{2}\operatorname{Re}\Big[((\overline{v^\varepsilon})^2)^2\cancelto{(1.4)}{(v^p_\varepsilon\delta v^\varepsilon_p)^2} - 2|v^\varepsilon|^2(\overline{v^\varepsilon})^2\cancelto{(2.5)}{(v^k_\varepsilon\delta v^\varepsilon_k)(\overline{v^p_\varepsilon\delta v^\varepsilon_p})} + (|v^\varepsilon|^2)^2\cancelto{(7.6)}{(\overline{v^k_\varepsilon\delta v^\varepsilon_k})^2} \\
&\qquad + (v^\varepsilon)^2(\overline{v^\varepsilon})^2\cancelto{(4.6)}{(v^k_\varepsilon\delta v^\varepsilon_k)(\overline{v^p_\varepsilon\delta v^\varepsilon_p})} - 2|v^\varepsilon|^2(\overline{v^\varepsilon})^2\cancelto{(5.7)}{(v^k_\varepsilon\delta v^\varepsilon_k)(\overline{v^p_\varepsilon\delta v^\varepsilon_p})} \\
&\qquad + (|v^\varepsilon|^2)^2\cancelto{(9.4)}{(\overline{v^k_\varepsilon\delta v^\varepsilon_k})(v^p_\varepsilon\delta v^\varepsilon_p)}\Big]\Bigg\} \\
&-\frac{8}{\mathcal{D}^\varepsilon}\Bigg\{-2\operatorname{Re}\Big[(\overline{v^\varepsilon})^2(\overline{s^\varepsilon})^2\cancelto{(1.5)}{(v^k_\varepsilon\delta v^\varepsilon_k)^2} - |v^\varepsilon|^2(\overline{s^\varepsilon})^2\cancelto{(2.6)}{(v^k_\varepsilon\delta v^\varepsilon_k)(\overline{v^p_\varepsilon\delta v^\varepsilon_p})} \\
&\qquad + (v^\varepsilon)^2(\overline{s^\varepsilon})^2\cancelto{(4.7)}{(v^k_\varepsilon\delta v^\varepsilon_k)(\overline{v^p_\varepsilon\delta v^\varepsilon_p})} - |v^\varepsilon|^2(\overline{s^\varepsilon})^2\cancelto{(5.8)}{(v^k_\varepsilon\delta v^\varepsilon_k)(\overline{v^p_\varepsilon\delta v^\varepsilon_p})} \\
&\qquad + (\overline{v^\varepsilon})^2|s^\varepsilon|^2\cancelto{(2.7)}{(\overline{v^k_\varepsilon\delta v^\varepsilon_k})(v^p_\varepsilon\delta v^\varepsilon_p)} - |v^\varepsilon|^2|s^\varepsilon|^2\cancelto{(7.7)}{(\overline{v^k_\varepsilon\delta v^\varepsilon_k})^2} \\
&\qquad + (v^\varepsilon)^2|s^\varepsilon|^2\cancelto{(5.9)}{(\overline{v^k_\varepsilon\delta v^\varepsilon_k})(\overline{v^p_\varepsilon\delta v^\varepsilon_p})} - |v^\varepsilon|^2|s^\varepsilon|^2\cancelto{(9.5)}{(\overline{v^k_\varepsilon\delta v^\varepsilon_k})(v^p_\varepsilon\delta v^\varepsilon_p)} \\
&\qquad + (\overline{v^\varepsilon})^2\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\cancelto{(3.3)}{\delta s^\varepsilon(v^p_\varepsilon\delta v^\varepsilon_p)} - |v^\varepsilon|^2\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\cancelto{(8.5)}{\delta s^\varepsilon(\overline{v^p_\varepsilon\delta v^\varepsilon_p})} \\
&\qquad + (v^\varepsilon)^2\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\cancelto{(6.5)}{\delta s^\varepsilon(\overline{v^p_\varepsilon\delta v^\varepsilon_p})} - |v^\varepsilon|^2\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\cancelto{(10.3)}{\delta s^\varepsilon(v^p_\varepsilon\delta v^\varepsilon_p)}\Big] \\
&\quad + \operatorname{Re}\Big[\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)\overline{s^\varepsilon}\cancelto{(2.8)}{(v^p_\varepsilon\delta v^\varepsilon_p)(\overline{v^k_\varepsilon\delta v^\varepsilon_k})} + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)s^\varepsilon\cancelto{(4.8)}{(v^p_\varepsilon\delta v^\varepsilon_p)(\overline{v^k_\varepsilon\delta v^\varepsilon_k})} \\
&\qquad + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)(\overline{v^\varepsilon})^2\cancelto{(3.4)}{(v^p_\varepsilon\delta v^\varepsilon_p)\delta s^\varepsilon} + \big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)|v^\varepsilon|^2\cancelto{(6.6)}{(v^p_\varepsilon\delta v^\varepsilon_p)\overline{\delta s^\varepsilon}} \\
&\qquad - \big(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon}\,\overline{s^\varepsilon}\big)\overline{s^\varepsilon}\cancelto{(7.8)}{(\overline{v^k_\varepsilon\delta v^\varepsilon_k})^2} - \big(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon}\,\overline{s^\varepsilon}\big)s^\varepsilon\cancelto{(5.10)}{(\overline{v^p_\varepsilon\delta v^\varepsilon_p})(\overline{v^k_\varepsilon\delta v^\varepsilon_k})} \\
&\qquad - \big(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon}\,\overline{s^\varepsilon}\big)(\overline{v^\varepsilon})^2\cancelto{(8.6)}{(\overline{v^p_\varepsilon\delta v^\varepsilon_p})\overline{\delta s^\varepsilon}} - \big(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon}\,\overline{s^\varepsilon}\big)|v^\varepsilon|^2\cancelto{(10.4)}{(\overline{v^p_\varepsilon\delta v^\varepsilon_p})\overline{\delta s^\varepsilon}} \\
&\qquad + \Big(\big(B^\varepsilon\overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)(v^\varepsilon)^2 - \big(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon}\,\overline{s^\varepsilon}\big)|v^\varepsilon|^2\Big)\times
\end{aligned}
$$

$$\times \Big(\cancelto{(14.5)}{\overline{s^\varepsilon}(\delta v^k_\varepsilon \delta \overline{v^\varepsilon_k})} + \cancelto{(13.5)}{s^\varepsilon(\delta \overline{v^k_\varepsilon} \delta \overline{v^\varepsilon_k})} + \cancelto{(6.7)}{(v^k_\varepsilon \delta \overline{v^\varepsilon_k}) \delta s^\varepsilon} + \cancelto{(8.7)}{(v^k_\varepsilon \delta \overline{v^\varepsilon_k}) \delta \overline{s^\varepsilon}} \Big) \Big] \Big\}$$

Combining and cancelling terms finally yields

$$\begin{aligned}
&\operatorname{Tr}\left(F^\varepsilon_\pm \delta A^\varepsilon F^\varepsilon_\mp \delta A^\varepsilon\right) = \\
&= -\frac{4}{\mathcal{D}^\varepsilon} \operatorname{Re}\Big[\underbrace{(C^\varepsilon)^2 (v^k_\varepsilon \delta v^\varepsilon_k)^2}_{(1.1)\,-\,(1.5)} - \underbrace{2B^\varepsilon C^\varepsilon (v^k_\varepsilon \delta v^\varepsilon_k)(\overline{v^k_\varepsilon} \delta v^\varepsilon_k)}_{(2.1)\,-\,(2.8)} \\
&\qquad - \underbrace{2C^\varepsilon \left(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\right)(v^k_\varepsilon \delta v^\varepsilon_k) \delta s^\varepsilon}_{(3.1)\,-\,(3.4)} + \underbrace{(B^\varepsilon)^2 (v^k_\varepsilon \delta v^\varepsilon_k)(\overline{v^k_\varepsilon} \delta \overline{v^\varepsilon_k})}_{(4.1)\,-\,(4.8)} \\
&\qquad - \underbrace{2B^\varepsilon C^\varepsilon (v^k_\varepsilon \delta v^\varepsilon_k)(v^k_\varepsilon \delta \overline{v^\varepsilon_k})}_{(5.1)\,-\,(5.10)} - \underbrace{2B^\varepsilon \left(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\right)(v^k_\varepsilon \delta v^\varepsilon_k) \delta \overline{s^\varepsilon}}_{(6.1)\,-\,(6.7)} \\
&\qquad + \underbrace{C^\varepsilon \overline{C^\varepsilon} (\overline{v^k_\varepsilon} \delta v^\varepsilon_k)^2}_{(7.1)\,-\,(7.8)} + \underbrace{2C^\varepsilon \left(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon}\,\overline{s^\varepsilon}\right)(\overline{v^k_\varepsilon} \delta v^\varepsilon_k) \delta s^\varepsilon}_{(8.1)\,-\,(8.7)} \\
&\qquad + \underbrace{(B^\varepsilon)^2 (\overline{v^k_\varepsilon} \delta v^\varepsilon_k)(v^k_\varepsilon \delta \overline{v^\varepsilon_k})}_{(9.1)\,-\,(9.5)} + \underbrace{2B^\varepsilon \left(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\right)(v^k_\varepsilon \delta \overline{v^\varepsilon_k}) \delta s^\varepsilon}_{(10.1)\,-\,(10.4)} \\
&\qquad + \underbrace{C^\varepsilon \left(|(v^\varepsilon)^2|^2 - (|v^\varepsilon|^2)^2\right)(\delta s^\varepsilon)^2}_{(11.1)\,-\,(11.3)} + \underbrace{B^\varepsilon \left(|(v^\varepsilon)^2|^2 - (|v^\varepsilon|^2)^2\right) \delta s^\varepsilon \delta \overline{s^\varepsilon}}_{(12.1)\,-\,(12.3)} \\
&\qquad + \underbrace{C^\varepsilon \mathcal{D}^\varepsilon (\delta v^k_\varepsilon \delta v^\varepsilon_k)}_{(13.1)\,-\,(13.5)} - \underbrace{B^\varepsilon \mathcal{D}^\varepsilon (\delta v^k_\varepsilon \delta \overline{v^\varepsilon_k})}_{(14.1)\,-\,(14.5)} \Big] \Big\}
\end{aligned} \tag{B.21}$$

(3) Conclusion

As the last step we insert the intermediate results (B.14) and (B.21) into (B.13) and thus find for the second variation of the eigenvalues

$$\begin{aligned}
\delta^2 \lambda^\varepsilon_\pm &\overset{(B.13)}{=} \frac{1}{2} \underbrace{\operatorname{Tr}\left[F^\varepsilon_\pm \delta^2 A^\varepsilon\right]}_{(B.14)} \pm \frac{1}{4\sqrt{\mathcal{D}^\varepsilon}} \underbrace{\operatorname{Tr}\left[F^\varepsilon_\pm \delta A^\varepsilon F^\varepsilon_\mp \delta A^\varepsilon\right]}_{(B.21)} \\
&\overset{(B.14)}{\underset{(B.21)}{=}} \operatorname{Re}\Big[2(\overline{v^i_\varepsilon} \delta^2 v^\varepsilon_i) + 2\overline{s^\varepsilon} \delta^2 s^\varepsilon + (\delta v^i_\varepsilon \delta \overline{v^\varepsilon_i}) + \delta s^\varepsilon \delta \overline{s^\varepsilon} \Big] \\
&\quad \pm \frac{1}{\sqrt{\mathcal{D}^\varepsilon}} \operatorname{Re}\Big[2B^\varepsilon (\overline{v^i_\varepsilon} \delta^2 v^\varepsilon_i) - 2C^\varepsilon (v^i_\varepsilon \delta^2 v^\varepsilon_i) + 2\big(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big) \delta^2 s^\varepsilon \\
&\qquad\qquad + 2\big(s^\varepsilon (\overline{v^i_\varepsilon} \delta v^\varepsilon_i) + \overline{s^\varepsilon} (v^i_\varepsilon \delta v^\varepsilon_i)\big) \delta \overline{s^\varepsilon} \\
&\qquad\qquad\quad - (v^i_\varepsilon \delta v^\varepsilon_j)(\overline{v^i_\varepsilon} \delta \overline{v^\varepsilon_i}) + (v^i_\varepsilon \delta \overline{v^\varepsilon_i})(\overline{v^j_\varepsilon} \delta v^\varepsilon_j) - C^\varepsilon (\delta v^k_\varepsilon \delta v^\varepsilon_k) + B^\varepsilon (\delta v^k_\varepsilon \delta \overline{v^\varepsilon_k}) \Big] \\
&\quad \mp \frac{1}{(\mathcal{D}^\varepsilon)^{3/2}} \operatorname{Re}\Big[(C^\varepsilon)^2 (v^k_\varepsilon \delta v^\varepsilon_k)^2 - 2B^\varepsilon C^\varepsilon (v^k_\varepsilon \delta v^\varepsilon_k)(\overline{v^k_\varepsilon} \delta v^\varepsilon_k) - 2B^\varepsilon C^\varepsilon (v^k_\varepsilon \delta v^\varepsilon_k)(v^k_\varepsilon \delta \overline{v^\varepsilon_k}) \\
&\qquad\qquad + (B^\varepsilon)^2 (v^k_\varepsilon \delta v^\varepsilon_k)(\overline{v^k_\varepsilon} \delta \overline{v^\varepsilon_k}) + C^\varepsilon \overline{C^\varepsilon} (\overline{v^k_\varepsilon} \delta v^\varepsilon_k)^2 + (B^\varepsilon)^2 (\overline{v^k_\varepsilon} \delta v^\varepsilon_k)(v^k_\varepsilon \delta \overline{v^\varepsilon_k}) \\
&\qquad\qquad - 2C^\varepsilon \big(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)(v^k_\varepsilon \delta v^\varepsilon_k) \delta s^\varepsilon + 2C^\varepsilon \big(B^\varepsilon s^\varepsilon + \overline{C^\varepsilon}\,\overline{s^\varepsilon}\big)(\overline{v^k_\varepsilon} \delta v^\varepsilon_k) \delta s^\varepsilon \\
&\qquad\qquad + 2B^\varepsilon \big(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)(v^k_\varepsilon \delta \overline{v^\varepsilon_k}) \delta s^\varepsilon - 2B^\varepsilon \big(B^\varepsilon \overline{s^\varepsilon} + C^\varepsilon s^\varepsilon\big)(v^k_\varepsilon \delta v^\varepsilon_k) \delta \overline{s^\varepsilon} \\
&\qquad\qquad + C^\varepsilon \big(|(v^\varepsilon)^2|^2 - (|v^\varepsilon|^2)^2\big)(\delta s^\varepsilon)^2 + B^\varepsilon \big(|(v^\varepsilon)^2|^2 - (|v^\varepsilon|^2)^2\big) \delta s^\varepsilon \delta \overline{s^\varepsilon} \Big]
\end{aligned}$$

This concludes the proof. □

C

Position Space Angular Integration

Contents

In this appendix we have collected the details of all the auxiliary calculations necessary to arrive at Lemma 4.2.5 (Position Space Angular Integration in (4.21)) in the main body in Subsection 4.2.1.

C.1 Conventions and Auxiliary Calculations

PROPOSITION C.1.1 (ANGULAR INTEGRATION OF EXPONENTIAL FACTOR)

For any $\vec{p} \in \mathbb{R}^3$ the integral of the exponential factor $\mathrm{e}^{\pm \mathrm{i}\vec{p}\cdot\vec{\xi}}$ with respect to the angular variables of $\vec{\xi}$ evaluates to

$$\int_{S^2} \mathrm{d}\Omega_\xi \; \mathrm{e}^{\mp \mathrm{i}\vec{p}\cdot\vec{\xi}} = 4\pi \frac{\sin(|\vec{p}|r)}{|\vec{p}|r} \overset{(4.26)}{=} 4\pi j_{0,1}(|\vec{p}|r) \tag{C.1}$$

Proof. For the computation of the integral

$$\int_{S^2} \mathrm{d}\Omega_\xi \; \mathrm{e}^{\mp \mathrm{i}\vec{p}\cdot\vec{\xi}}$$

we choose, without loss of generality, a Cartesian coordinate system such that its z-axis points in the direction of $\vec{p}$. As a consequence, the scalar product $\vec{p}\cdot\vec{\xi}$ can be expressed as

$$\vec{p}\cdot\vec{\xi} = |\vec{p}||\vec{\xi}|\cos(\theta_\xi)$$

where θ_ξ denotes the angle between $\vec{\xi}$ and the z-axis. Splitting $\mathrm{d}\Omega_\xi$ into azimuthal and polar parts and defining $r := |\vec{\xi}|$, we obtain

$$\int_{S^2} \mathrm{d}\Omega_\xi \; \mathrm{e}^{\mp\mathrm{i}\vec{p}\cdot\vec{\xi}} = \int_{-1}^{1} \mathrm{d}\cos(\theta_\xi) \int_{0}^{2\pi} \mathrm{d}\varphi_\xi \; \mathrm{e}^{\mp\mathrm{i}|\vec{p}|r\cos(\theta_\xi)} = 2\pi \int_{-1}^{1} \mathrm{d}\cos(\theta_\xi) \; \mathrm{e}^{\mp\mathrm{i}|\vec{p}|r\cos(\theta_\xi)}$$

where in the last step we used the fact that the azimuthal integral can be carried out trivially due to the absence of any dependences on φ_ξ. Computing the remaining integral, we finally end up with

$$\int_{S^2} \mathrm{d}\Omega_\xi \; \mathrm{e}^{\mp\mathrm{i}\vec{p}\cdot\vec{\xi}} = 2\pi\left[\frac{\mathrm{e}^{\mp\mathrm{i}|\vec{p}|r}}{\mp\mathrm{i}|\vec{p}|r} - \frac{\mathrm{e}^{\pm\mathrm{i}|\vec{p}|r}}{\mp\mathrm{i}|\vec{p}|r}\right] = \mp 4\pi \frac{\sin(\mp|\vec{p}|r)}{|\vec{p}|r} \overset{(4.26)}{=} 4\pi j_{0,1}(|\vec{p}|r)$$

which concludes the proof. □

In the rest of this appendix, the generalized spherical bessel functions will almost exclusively appear with the argument $|\vec{p}\pm\vec{q}|r$. For notational convenience we therefore introduce the function $k_\pm : \mathbb{R}^3\times\mathbb{R}^3 \to \mathbb{R}_0^+$ defined as $k_\pm(\vec{p},\vec{q}) := |\vec{p}\pm\vec{q}|$. Whenever there is no risk of confusion, we suppress the arguments of the function $k_\pm$ such that, unless otherwise stated, any appearance of $k_\pm r$ must be understood as $|\vec{p}\pm\vec{q}|r$.

Convention C.1.2 (Arguments of Spherical Harmonics)

For the sake of notational clarity, we suppress arguments of spherical harmonics whenever there is no risk of confusion. We use the convention that scalar and vector spherical harmonics with unprimed parameters lm come with arguments (θ_p, φ_p) while scalar and vector spherical harmonics with primed parameters $l'm'$ always carry arguments (θ_q, φ_q).

C.1.1 Basic Derivatives of $j_{0,n}(k_\pm r)$

In the proofs of Lemma C.2.1 and Lemma C.4.1, various derivatives of $j_{0,n}(k_\pm r)$ enter the game. In order to keep these proofs as compact as possible, we outsource the computation of derivatives and collect them in the following proposition.

Proposition C.1.3 (First and Second Derivatives of $j_{0,n}(k_\pm r)$)

The first derivatives of $j_{0,n}(k_\pm r)$, namely the gradients with respect to $\vec{p}$, $\vec{q}$ and the derivatives with respect to $|\vec{p}|$, $|\vec{q}|$, are given by

$$\begin{Bmatrix} \mathrm{grad}_{\vec{p}}\, j_{0,n}(k_\pm r) \\ \mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) \end{Bmatrix} = \begin{Bmatrix} 1 \\ \pm 1 \end{Bmatrix} 2(\vec{p}\pm\vec{q})r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n+2}(k_\pm r) \tag{C.2a}$$

$$\begin{Bmatrix} \vec{p}\cdot\mathrm{grad}_{\vec{p}}\, j_{0,n}(k_\pm r) \\ \vec{q}\cdot\mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) \end{Bmatrix} = \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} j_{0,n}(k_\pm r) + \begin{Bmatrix} +1 \\ -1 \end{Bmatrix} (|\vec{p}|^2 - |\vec{q}|^2) r^2 \left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n+2}(k_\pm r) \tag{C.2b}$$

$$\begin{Bmatrix} \vec{q}\cdot \mathrm{grad}_{\vec{p}}\, j_{0,n}(k_\pm r) \\ \vec{p}\cdot \mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) \end{Bmatrix} = \pm\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} j_{0,n}(k_\pm r) \pm \begin{Bmatrix} -1 \\ +1 \end{Bmatrix} (|\vec{p}|^2 - |\vec{q}|^2) r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n+2}(k_\pm r) \tag{C.2c}$$

$$\begin{Bmatrix} |\vec{p}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{p}|} \\ |\vec{q}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{q}|} \end{Bmatrix} = \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} j_{0,n}(k_\pm r) + \begin{Bmatrix} +1 \\ -1 \end{Bmatrix} (|\vec{p}|^2 - |\vec{q}|^2) r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n+2}(k_\pm r) \tag{C.2d}$$

The second-order derivatives, namely the divergence and curl of the gradients as well as the mixed derivatives with respect to $|\vec{p}|$ and $|\vec{q}|$ read

$$\begin{Bmatrix} \mathrm{div}_{\vec{q}}\, \mathrm{grad}_{\vec{p}}\, j_{0,n}(k_\pm r) \\ \mathrm{div}_{\vec{p}}\, \mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) \end{Bmatrix} = \pm 4r^2 \left[\frac{3}{2} + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n+2}(k_\pm r) \tag{C.3a}$$

$$\begin{Bmatrix} \mathrm{curl}_{\vec{q}}\, \mathrm{grad}_{\vec{p}}\, j_{0,n}(k_\pm r) \\ \mathrm{curl}_{\vec{p}}\, \mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) \end{Bmatrix} = \vec{0} \tag{C.3b}$$

$$\begin{aligned} |\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}|\vec{q}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{q}|} &= \left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 j_{0,n}(k_\pm r) - (|\vec{p}|^2 + |\vec{q}|^2) r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n+2}(k_\pm r) \\ &\quad - (|\vec{p}|^2 - |\vec{q}|^2)^2 r^4 \left[2 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n+4}(k_\pm r) \end{aligned} \tag{C.3c}$$

Proof. To prove the above relations we will repeatedly make use of the identities

$$\vec{p}\cdot(\vec{p}\pm\vec{q}) = \frac{k_\pm^2 + |\vec{p}|^2 - |\vec{q}|^2}{2} \tag{C.4a}$$

$$\vec{q}\cdot(\vec{p}\pm\vec{q}) = \pm\frac{k_\pm^2 - |\vec{p}|^2 + |\vec{q}|^2}{2} \tag{C.4b}$$

as well as

$$\mathrm{grad}_{\vec{p}}\, k_\pm = \frac{\vec{p}\pm\vec{q}}{k_\pm} \tag{C.5a}$$

$$\mathrm{grad}_{\vec{q}}\, k_\pm = \pm\frac{\vec{p}\pm\vec{q}}{k_\pm} \tag{C.5b}$$

which immediately follow by straightforward computation and remembering that $k_\pm = |\vec{p}\pm\vec{q}|$.

(1) First Derivatives of $j_{0,n}(k_\pm r)$

Making use of these identities we find the following expressions for the gradients of $j_{0,n}(k_\pm r)$ with respect to $\vec{p}$ and $\vec{q}$, respectively

$$\begin{aligned} \mathrm{grad}_{\vec{p}}\, j_{0,n}(k_\pm r) &= \frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}k_\pm}\mathrm{grad}_{\vec{p}}\, k_\pm \overset{\text{(C.5a)}}{=} \frac{r}{k_\pm}\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}r}\frac{\vec{p}\pm\vec{q}}{k_\pm} \\ &\overset{\text{(4.26)}}{=} (\vec{p}\pm\vec{q}) r \frac{\mathrm{d}\big(r^2 j_{0,n+2}(k_\pm r)\big)}{\mathrm{d}r} = 2(\vec{p}\pm\vec{q}) r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n+2}(k_\pm r) \end{aligned} \tag{C.6}$$

$$\begin{aligned} \mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) &= \frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}k_\pm}\mathrm{grad}_{\vec{q}}\, k_\pm \overset{\text{(C.5b)}}{=} \pm\frac{r}{k_\pm}\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}r}\frac{\vec{p}\pm\vec{q}}{k_\pm} \\ &\overset{\text{(4.26)}}{=} \pm(\vec{p}\pm\vec{q}) r \frac{\mathrm{d}\big(r^2 j_{0,n+2}(k_\pm r)\big)}{\mathrm{d}r} = \pm 2(\vec{p}\pm\vec{q}) r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n+2}(k_\pm r) \end{aligned} \tag{C.7}$$

Due to the fact that gradients often occur in scalar products with $\vec{p}$ and $\vec{q}$, we also compute these expressions. For the scalar products of $\mathrm{grad}_{\vec{p}}\, j_{0,n}$ and $\mathrm{grad}_{\vec{q}}\, j_{0,n}$ with the corresponding momentum vectors $\vec{p}$ and $\vec{q}$ we find

$$\begin{aligned}
\vec{p}\cdot\mathrm{grad}_{\vec{p}}\, j_{0,n}(k_\pm r) &\overset{(C.6)}{=} 2\vec{p}\cdot(\vec{p}\pm\vec{q})r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\\
&= \left(k_\pm^2+|\vec{p}|^2-|\vec{q}|^2\right)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\\
&\overset{(4.26)}{=} r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left(r^{-2}j_{0,n}(k_\pm r)\right)+(|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\\
&= \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r)+(|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)
\end{aligned} \tag{C.8}$$

$$\begin{aligned}
\vec{q}\cdot\mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) &\overset{(C.7)}{=} \pm 2\vec{q}\cdot(\vec{p}\pm\vec{q})r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\\
&= \left(k_\pm^2-|\vec{p}|^2+|\vec{q}|^2\right)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\\
&\overset{(4.26)}{=} r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left(r^{-2}j_{0,n}(k_\pm r)\right)-(|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\\
&= \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r)-(|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)
\end{aligned} \tag{C.9}$$

For the mixed expressions we analogously find

$$\begin{aligned}
\vec{q}\cdot\mathrm{grad}_{\vec{p}}\, j_{0,n}(k_\pm r) &\overset{(C.7)}{=} 2\vec{q}\cdot(\vec{p}\pm\vec{q})r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\\
&= \pm\left(k_\pm^2-|\vec{p}|^2+|\vec{q}|^2\right)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\\
&\overset{(4.26)}{=} \pm r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left(r^{-2}j_{0,n}(k_\pm r)\right)\mp(|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\\
&= \pm\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r)\mp(|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)
\end{aligned} \tag{C.10}$$

$$\begin{aligned}
\vec{p}\cdot\mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) &\overset{(C.7)}{=} \pm 2\vec{p}\cdot(\vec{p}\pm\vec{q})r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\\
&= \pm\left(k_\pm^2+|\vec{p}|^2-|\vec{q}|^2\right)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\\
&\overset{(4.26)}{=} \pm r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left(r^{-2}j_{0,n}(k_\pm r)\right)\pm(|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\\
&= \pm\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r)\pm(|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)
\end{aligned} \tag{C.11}$$

Next, we turn to the computation of derivatives of $j_{0,n}(k_\pm r)$ with respect to $|\vec{p}|$ and $|\vec{q}|$. For this we need the relations

$$\begin{aligned}
|\vec{p}|\frac{\mathrm{d}k_\pm}{\mathrm{d}|\vec{p}|} &= \frac{|\vec{p}|}{2k_\pm}\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\left[|\vec{p}|^2+|\vec{q}|^2\pm 2|\vec{p}||\vec{q}|\cos\left(\sphericalangle(\hat{\vec{e}}_p,\hat{\vec{e}}_q)\right)\right]\\
&= |\vec{p}|\frac{|\vec{p}|\pm|\vec{q}|\cos\left(\sphericalangle(\hat{\vec{e}}_p,\hat{\vec{e}}_q)\right)}{k_\pm} = \frac{k_\pm^2+|\vec{p}|^2-|\vec{q}|^2}{2k_\pm} \qquad \text{(C.12)}\\
|\vec{q}|\frac{\mathrm{d}k_\pm}{\mathrm{d}|\vec{q}|} &= \frac{|\vec{q}|}{2k_\pm}\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[|\vec{p}|^2+|\vec{q}|^2\pm 2|\vec{p}||\vec{q}|\cos\left(\sphericalangle(\hat{\vec{e}}_p,\hat{\vec{e}}_q)\right)\right]
\end{aligned}$$

$$= |\vec{q}|\frac{|\vec{q}| \pm |\vec{p}|\cos\left(\sphericalangle(\hat{\vec{e}}_p, \hat{\vec{e}}_q)\right)}{k_\pm} = \frac{k_\pm^2 - (|\vec{p}|^2 - |\vec{q}|^2)}{2k_\pm} \tag{C.13}$$

where we used $\vec{p}\cdot\vec{q} = |\vec{p}||\vec{q}|\cos(\sphericalangle(\hat{\vec{e}}_p, \hat{\vec{e}}_q))$ with $\sphericalangle(\hat{\vec{e}}_p, \hat{\vec{e}}_q)$ denoting the angle between the unit vectors $\hat{\vec{e}}_p$ and $\hat{\vec{q}}$ pointing in directions of $\vec{p}$ and $\vec{q}$, respectively. Using this we find

$$\begin{aligned}
|\vec{p}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{p}|} &= \frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}k_\pm}|\vec{p}|\frac{\mathrm{d}k_\pm}{\mathrm{d}|\vec{p}|} \overset{\text{(C.12)}}{=} \frac{r}{k_\pm}\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}r}\frac{k_\pm^2 + |\vec{p}|^2 - |\vec{q}|^2}{2k_\pm} \\
&\overset{\text{(4.26)}}{=} \frac{r}{2}\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}r} + \frac{r}{2}(|\vec{p}|^2 - |\vec{q}|^2)\frac{\mathrm{d}\big(r^2 j_{0,n+2}(k_\pm r)\big)}{\mathrm{d}r} \\
&= \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r) + r^2(|\vec{p}|^2 - |\vec{q}|^2)\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)
\end{aligned} \tag{C.14}$$

$$\begin{aligned}
|\vec{q}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{q}|} &= \frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}k_\pm}|\vec{q}|\frac{\mathrm{d}k_\pm}{\mathrm{d}|\vec{q}|} \overset{\text{(C.13)}}{=} \frac{r}{k_\pm}\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}r}\frac{k_\pm^2 - (|\vec{p}|^2 - |\vec{q}|^2)}{2k_\pm} \\
&\overset{\text{(4.26)}}{=} \frac{r}{2}\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}r} - \frac{r}{2}(|\vec{p}|^2 - |\vec{q}|^2)\frac{\mathrm{d}\big(r^2 j_{0,n+2}(k_\pm r)\big)}{\mathrm{d}r} \\
&= \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r) - r^2(|\vec{p}|^2 - |\vec{q}|^2)\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)
\end{aligned} \tag{C.15}$$

(2) Second Derivatives of $j_{0,n}(k_\pm r)$

For the second derivatives of $j_{0,n}(k_\pm r)$ there are various combinations possible. Taking the gradients as our starting point, we can compute their divergence as well as their curl. For the former we find

$$\begin{aligned}
&\mathrm{div}_{\vec{q}}\ \mathrm{grad}_{\vec{p}}\, j_{0,n}(k_\pm r) = \\
&\overset{\text{(C.6)}}{=} \mathrm{div}_{\vec{q}}\left(2(\vec{p} \pm \vec{q})r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\right) \\
&= \pm 6r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r) + 2r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right](\vec{p} \pm \vec{q})\cdot\mathrm{grad}_{\vec{q}}\, j_{0,n+2}(k_\pm r) \\
&\overset{\text{(C.5b)}}{\underset{\text{(4.26)}}{=}} \pm 6r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r) \pm 4r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left(r^{-2}j_{0,n+2}(k_\pm r)\right)\right] \\
&= \pm 6r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r) \pm 4r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r) \\
&= \pm 4r^2\left[\frac{3}{2} + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)
\end{aligned} \tag{C.16}$$

$$\begin{aligned}
&\mathrm{div}_{\vec{p}}\ \mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) = \\
&\overset{\text{(C.7)}}{=} \mathrm{div}_{\vec{p}}\left(\pm 2(\vec{p} \pm \vec{q})r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\right) \\
&= \pm 6r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r) \pm 2r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right](\vec{p} \pm \vec{q})\cdot\mathrm{grad}_{\vec{p}}\, j_{0,n+2}(k_\pm r) \\
&\overset{\text{(C.5a)}}{\underset{\text{(4.26)}}{=}} \pm 6r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r) \pm 4r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left(r^{-2}j_{0,n+2}(k_\pm r)\right)\right] \\
&\overset{\text{(C.16)}}{=} \mathrm{div}_{\vec{q}}\ \mathrm{grad}_{\vec{p}}\, j_{0,n}(k_\pm r)
\end{aligned} \tag{C.17}$$

Repeating the procedure for the curl gives

$$\begin{aligned}
\operatorname{curl}_{\vec{q}}\, \operatorname{grad}_{\vec{p}}\, j_{0,n}(k_\pm r) &\overset{(C.6)}{=} \operatorname{curl}_{\vec{q}} \left(2(\vec{p} \pm \vec{q}) r^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] j_{0,n+2}(k_\pm r) \right) \\
&= 2r^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] \big(\operatorname{grad}_{\vec{q}}\, j_{0,n+2}(k_\pm r) \big) \times (\vec{p} \pm \vec{q}) \\
&\overset{(C.7)}{=} \pm 2r^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] \left[2r^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] j_{0,n+4}(k_\pm r) \right] (\vec{p} \pm \vec{q}) \times (\vec{p} \pm \vec{q}) \\
&= \vec{0}
\end{aligned} \tag{C.18}$$

$$\begin{aligned}
\operatorname{curl}_{\vec{p}}\, \operatorname{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) &\overset{(C.7)}{=} \operatorname{curl}_{\vec{p}} \left(\pm 2(\vec{p} \pm \vec{q}) r^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] j_{0,n+2}(k_\pm r) \right) \\
&= \pm 2r^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] \big(\operatorname{grad}_{\vec{p}}\, j_{0,n+2}(k_\pm r) \big) \times (\vec{p} \pm \vec{q}) \\
&\overset{(C.6)}{=} \pm 2r^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] \left[2r^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] j_{0,n+4}(k_\pm r) \right] (\vec{p} \pm \vec{q}) \times (\vec{p} \pm \vec{q}) \\
&= \vec{0}
\end{aligned} \tag{C.19}$$

Here we used the rules for the curl as well as the properties of the cross product. Finally, for mixed derivatives with respect to $|\vec{p}|$ and $|\vec{q}|$ we find

$$\begin{aligned}
&|\vec{p}| \frac{\mathrm{d}}{\mathrm{d}|\vec{p}|} |\vec{q}| \frac{\mathrm{d} j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{q}|} = \\
&\overset{(C.13)}{=} |\vec{p}| \frac{\mathrm{d}}{\mathrm{d}|\vec{p}|} \left[\frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} j_{0,n}(k_\pm r) - r^2 (|\vec{p}|^2 - |\vec{q}|^2) \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] j_{0,n+2}(k_\pm r) \right] \\
&\overset{(C.12)}{=} \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \left[\frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} j_{0,n}(k_\pm r) + r^2 (|\vec{p}|^2 - |\vec{q}|^2) \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] j_{0,n+2}(k_\pm r) \right] \\
&\quad - 2r^2 |\vec{p}|^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] j_{0,n+2}(k_\pm r) \\
&\quad - r^2 (|\vec{p}|^2 - |\vec{q}|^2) \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] \left[\frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} j_{0,n+2}(k_\pm r) + r^2 (|\vec{p}|^2 - |\vec{q}|^2) \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] j_{0,n+4}(k_\pm r) \right] \\
&= \left[\frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right]^2 j_{0,n}(k_\pm r) - (|\vec{p}|^2 + |\vec{q}|^2) r^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] j_{0,n+2}(k_\pm r) \\
&\quad - (|\vec{p}|^2 - |\vec{q}|^2)^2 \left[r^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] \right]^2 j_{0,n+4}(k_\pm r) \\
&= \left[\frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right]^2 j_{0,n}(k_\pm r) - (|\vec{p}|^2 + |\vec{q}|^2) r^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] j_{0,n+2}(k_\pm r) \\
&\quad - (|\vec{p}|^2 - |\vec{q}|^2)^2 r^4 \left[2 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] j_{0,n+4}(k_\pm r)
\end{aligned} \tag{C.20}$$

This concludes the proof. □

C.1.2 Auxiliary Calculations

In this subsection we collect auxiliary calculations which are needed in order to simplify intermediate results appearing in Appendix Section C.2, Appendix Section C.3 and Appendix Section C.4. Being straightforward though non-obvious calculations, they do not deserve the status of propositions and thus come mainly without any further explanatory comments.

C.1.2.1 Auxiliary Calculations for Dotted-Primed/Unprimed Terms

Auxiliary Calculation C.1.4 ((C.36) in Lemma C.2.1)

$$\begin{Bmatrix} -\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\left[|\vec{p}|\vec{p}\cdot\vec{q}\,j_{0,3}(k_\pm r)\right] + |\vec{p}|^2\vec{q}\cdot\mathrm{grad}_{\vec{p}}\,j_{0,3}(k_\pm r) \\ -\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[|\vec{q}|\vec{p}\cdot\vec{q}\,j_{0,3}(k_\pm r)\right] + |\vec{q}|^2\vec{p}\cdot\mathrm{grad}_{\vec{q}}\,j_{0,3}(k_\pm r) \end{Bmatrix} =$$

$$= \mp\frac{1}{2r^2}\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,1}(k_\pm r) \pm (|\vec{p}|^2+|\vec{q}|^2)\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,3}(k_\pm r) \mp \frac{(|\vec{p}|^2-|\vec{q}|^2)^2}{2}r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,5}(k_\pm r) \tag{C.21}$$

Proof.

$$\begin{aligned}
&-\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\left[|\vec{p}|\vec{p}\cdot\vec{q}\,j_{0,3}(k_\pm r)\right] + |\vec{p}|^2\vec{q}\cdot\mathrm{grad}_{\vec{p}}\,j_{0,3}(k_\pm r) = \\
&\quad= \mp\frac{1}{2}\left(k_\pm^2-|\vec{p}|^2-|\vec{q}|^2\right)j_{0,3}(k_\pm r) \\
&\qquad\mp |\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\left(\frac{1}{2}\left(k_\pm^2-|\vec{p}|^2-|\vec{q}|^2\right)j_{0,3}(k_\pm r)\right) + |\vec{p}|^2\vec{q}\cdot\mathrm{grad}_{\vec{p}}\,j_{0,3}(k_\pm r) \\
&\quad\overset{(4.26)}{=} \mp\frac{1}{2r^2}j_{0,1}(k_\pm r) \pm \frac{|\vec{p}|^2+|\vec{q}|^2}{2}j_{0,3}(k_\pm r) \mp \frac{1}{2r^2}|\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}j_{0,1}(k_\pm r) \\
&\qquad\pm |\vec{p}|^2 j_{0,3}(k_\pm r) \pm \frac{|\vec{p}|^2+|\vec{q}|^2}{2}|\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}j_{0,3}(k_\pm r) + |\vec{p}|^2\vec{q}\cdot\mathrm{grad}_{\vec{p}}\,j_{0,3}(k_\pm r) \\
&\quad\underset{(C.2d)}{\overset{(C.2c)}{=}} \mp\frac{1}{2r^2}j_{0,1}(k_\pm r) \pm \frac{|\vec{p}|^2+|\vec{q}|^2}{2}j_{0,3}(k_\pm r) \\
&\qquad\mp \frac{1}{2r^2}\left(\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,1}(k_\pm r) + (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,3}(k_\pm r)\right) \\
&\qquad\pm |\vec{p}|^2 j_{0,3}(k_\pm r) \pm \frac{|\vec{p}|^2+|\vec{q}|^2}{2}\left(\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,3}(k_\pm r) + (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,5}(k_\pm r)\right) \\
&\qquad\pm |\vec{p}|^2\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,3}(k_\pm r) - (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,5}(k_\pm r)\right] \\
&\quad= \mp\frac{1}{2r^2}\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,1}(k_\pm r) \pm (|\vec{p}|^2+|\vec{q}|^2)\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,3}(k_\pm r) \\
&\qquad\mp \frac{(|\vec{p}|^2-|\vec{q}|^2)^2}{2}r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,5}(k_\pm r)
\end{aligned} \tag{C.22}$$

$$\begin{aligned}
&-\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[|\vec{q}|\vec{p}\cdot\vec{q}\,j_{0,3}(k_\pm r)\right] + |\vec{q}|^2\vec{p}\cdot\mathrm{grad}_{\vec{q}}\,j_{0,3}(k_\pm r) = \\
&\quad= \mp\frac{1}{2}\left(k_\pm^2-|\vec{p}|^2-|\vec{q}|^2\right)j_{0,3}(k_\pm r) \\
&\qquad\mp |\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left(\frac{1}{2}\left(k_\pm^2-|\vec{p}|^2-|\vec{q}|^2\right)j_{0,3}(k_\pm r)\right) + |\vec{q}|^2\vec{p}\cdot\mathrm{grad}_{\vec{q}}\,j_{0,3}(k_\pm r) \\
&\quad\overset{(4.26)}{=} \mp\frac{1}{2r^2}j_{0,1}(k_\pm r) \pm \frac{|\vec{p}|^2+|\vec{q}|^2}{2}j_{0,3}(k_\pm r) \mp \frac{1}{2r^2}|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}j_{0,1}(k_\pm r) \\
&\qquad\pm |\vec{q}|^2 j_{0,3}(k_\pm r) \pm \frac{|\vec{p}|^2+|\vec{q}|^2}{2}|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}j_{0,3}(k_\pm r) + |\vec{q}|^2\vec{p}\cdot\mathrm{grad}_{\vec{q}}\,j_{0,3}(k_\pm r)
\end{aligned}$$

$$
\begin{aligned}
&\overset{\text{(C.2c)}}{\underset{\text{(C.2d)}}{=}} \mp \frac{1}{2r^2} j_{0,1}(k_\pm r) \pm \frac{|\vec{p}|^2 + |\vec{q}|^2}{2} j_{0,3}(k_\pm r) \\
&\quad \mp \frac{1}{2r^2}\left(\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} j_{0,1}(k_\pm r) - (|\vec{p}|^2 - |\vec{q}|^2) r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,3}(k_\pm r)\right) \\
&\quad \pm |\vec{q}|^2 j_{0,3}(k_\pm r) \pm \frac{|\vec{p}|^2 + |\vec{q}|^2}{2}\left(\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} j_{0,3}(k_\pm r) - (|\vec{p}|^2 - |\vec{q}|^2) r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,5}(k_\pm r)\right) \\
&\quad \pm |\vec{q}|^2 \left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} j_{0,3}(k_\pm r) + (|\vec{p}|^2 - |\vec{q}|^2) r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,5}(k_\pm r)\right] \\
&= \mp \frac{1}{2r^2}\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,1}(k_\pm r) \pm (|\vec{p}|^2 + |\vec{q}|^2)\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,3}(k_\pm r) \\
&\quad \mp \frac{(|\vec{p}|^2 - |\vec{q}|^2)^2}{2} r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,5}(k_\pm r)
\end{aligned} \tag{C.23}
$$

This concludes the proof. □

C.1.2.2 Auxiliary Calculations for Double-Dotted Terms

Auxiliary Calculation C.1.5 ((C.44) in Lemma C.3.1)

$$
\begin{aligned}
\left(\vec{p}\cdot \mathrm{grad}_{\vec{p}}\right)\left(\vec{q}\cdot \mathrm{grad}_{\vec{q}}\right) j_{0,1}(k_\pm r) &= \left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 j_{0,1}(k_\pm r) - (|\vec{p}|^2 + |\vec{q}|^2) r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,3}(k_\pm r) \\
&\quad - (|\vec{p}|^2 - |\vec{q}|^2)^2 r^4 \left[2 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,5}(k_\pm r)
\end{aligned} \tag{C.24}
$$

Proof. To show the claimed relation we first insert (C.2b) for the gradient with respect to $\vec{q}$ and thus obtain

$$
\begin{aligned}
&\left(\vec{p}\cdot \mathrm{grad}_{\vec{p}}\right)\left(\vec{q}\cdot \mathrm{grad}_{\vec{q}}\right) j_{0,1}(k_\pm r) = \\
&\overset{\text{(C.2b)}}{=} \left(\vec{p}\cdot \mathrm{grad}_{\vec{p}}\right)\left(\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} j_{0,1}(k_\pm r) - (|\vec{p}|^2 - |\vec{q}|^2) r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,3}(k_\pm r)\right)
\end{aligned}
$$

Carrying out the gradient with respect to $\vec{p}$ results in

$$
\begin{aligned}
\cdots = \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\vec{p}\cdot \mathrm{grad}_{\vec{p}}\, j_{0,1}(k_\pm r) - 2|\vec{p}|^2 r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,3}(k_\pm r) \\
- (|\vec{p}|^2 - |\vec{q}|^2) r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \vec{p}\cdot \mathrm{grad}_{\vec{p}}\, j_{0,3}(k_\pm r)
\end{aligned}
$$

Using (C.2b) for a second time turns the expression into the form

$$
\begin{aligned}
\ldots &\overset{\text{(C.2b)}}{=} \left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 j_{0,1}(k_\pm r) + (|\vec{p}|^2 - |\vec{q}|^2)\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[r^2 + \frac{r^3}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,3}(k_\pm r) \\
&\quad - 2|\vec{p}|^2 r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,3}(k_\pm r) - (|\vec{p}|^2 - |\vec{q}|^2) r^2 \left[\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} j_{0,3}(k_\pm r)\right. \\
&\quad \left. + (|\vec{p}|^2 - |\vec{q}|^2)\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[r^2 + \frac{r^3}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,5}(k_\pm r)\right]
\end{aligned}
$$

By collecting terms we finally end up with

$$\cdots = \left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 j_{0,1}(k_\pm r) - (|\vec{p}|^2 + |\vec{q}|^2)r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,3}(k_\pm r)$$
$$- (|\vec{p}|^2 - |\vec{q}|^2)^2 r^4\left[2 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,5}(k_\pm r)$$

This concludes the proof. □

C.1.2.3 Auxiliary Calculations for Asterisked Terms

For the position space integration of asterisked terms, i. e. terms where two vector spherical harmonics are contracted with each other[1], calculations become rather lengthy. Especially in the cases $\vec{\Psi}_{lm}(\theta_p, \varphi_p) \cdot \vec{\Psi}_{l'm'}(\theta_q, \varphi_q)$ and $\vec{\Phi}_{lm}(\theta_p, \varphi_p) \cdot \vec{\Phi}_{l'm'}(\theta_q, \varphi_q)$ the necessity to evaluate complicated derivatives arises in the course of the calculations.

Auxiliary Calculation C.1.6 (Integrand of $\vec{Y}_{lm} \cdot \vec{\Psi}_{l'm'}$ in (C.54) in Lemma C.4.1)

$$\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\Big[(\vec{p}\cdot\vec{q})|\vec{q}|j_{0,1}(k_\pm r)\Big] - |\vec{q}|^2\vec{p}\cdot\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) =$$
$$= \pm\frac{1}{2r^2}\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,-1}(k_\pm r) \mp (|\vec{p}|^2 + |\vec{q}|^2)\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,1}(k_\pm r)$$
$$\pm \frac{(|\vec{p}|^2 - |\vec{q}|^2)^2}{2}r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,3}(k_\pm r) \tag{C.25}$$

Proof.

$$\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\Big[(\vec{p}\cdot\vec{q})|\vec{q}|j_{0,1}(k_\pm r)\Big] - |\vec{q}|^2\vec{p}\cdot\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) =$$
$$= (\vec{p}\cdot\vec{q})j_{0,1}(k_\pm r) + |\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\Big[(\vec{p}\cdot\vec{q})j_{0,1}(k_\pm r)\Big] - |\vec{q}|^2\vec{p}\cdot\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)$$
$$= \pm\frac{k_\pm^2 - (|\vec{p}|^2 + |\vec{q}|^2)}{2}j_{0,1}(k_\pm r)$$
$$+ |\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[\pm\frac{k_\pm^2 - (|\vec{p}|^2 + |\vec{q}|^2)}{2}j_{0,1}(k_\pm r)\right] - |\vec{q}|^2\vec{p}\cdot\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)$$
$$\overset{(4.26)}{=} \pm\frac{1}{2r^2}j_{0,-1}(k_\pm r) \mp \frac{|\vec{p}|^2 + |\vec{q}|^2}{2}j_{0,1}(k_\pm r)$$
$$\pm |\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[\frac{1}{2r^2}j_{0,-11}(k_\pm r) - \frac{|\vec{p}|^2 + |\vec{q}|^2}{2}j_{0,1}(k_\pm r)\right] - |\vec{q}|^2\vec{p}\cdot\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)$$
$$= \pm\frac{1}{2r^2}j_{0,-11}(k_\pm r) \mp \frac{|\vec{p}|^2 + |\vec{q}|^2}{2}j_{0,1}(k_\pm r) \pm \frac{1}{2r^2}|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}j_{0,-11}(k_\pm r)$$
$$\mp |\vec{q}|^2 j_{0,1}(k_\pm r) - \frac{|\vec{p}|^2 + |\vec{q}|^2}{2}|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}j_{0,1}(k_\pm r) - |\vec{q}|^2\vec{p}\cdot\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)$$
$$\overset{(C.2c)}{\underset{(C.2d)}{=}} \pm\frac{1}{2r^2}j_{0,-1}(k_\pm r) \mp \frac{|\vec{p}|^2 + |\vec{q}|^2}{2}j_{0,1}(k_\pm r)$$

[1] For the definition of asterisked terms, recall Terminology 4.1.7.

$$\pm \frac{1}{2r^2}\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} j_{0,-1}(k_\pm r) - (|\vec{p}|^2 - |\vec{q}|^2) r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,1}(k_\pm r)\right] \mp |\vec{q}|^2 j_{0,1}(k_\pm r)$$
$$\mp \frac{|\vec{p}|^2 + |\vec{q}|^2}{2}\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} j_{0,1}(k_\pm r) - (|\vec{p}|^2 - |\vec{q}|^2) r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,3}(k_\pm r)\right]$$
$$- |\vec{q}|^2 \left[\pm \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} j_{0,1}(k_\pm r) \pm (|\vec{p}|^2 - |\vec{q}|^2) r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,3}(k_\pm r)\right]$$
$$= \pm \frac{1}{2r^2}\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,-1}(k_\pm r) \mp (|\vec{p}|^2 + |\vec{q}|^2)\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,1}(k_\pm r)$$
$$\pm \frac{(|\vec{p}|^2 - |\vec{q}|^2)^2}{2} r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,3}(k_\pm r) \qquad \text{(C.26)}$$

This concludes the proof. □

AUXILIARY CALCULATION C.1.7 (INTEGRAND OF $\vec{\Psi}_{lm} \cdot \vec{\Psi}_{l'm'}$ IN (C.56) IN LEMMA C.4.1)

$$\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\left[|\vec{p}|(\vec{p}\cdot\vec{q}) j_{0,n}(k_\pm r)\right]\right] - |\vec{p}|^2 \frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[|\vec{q}|\vec{q}\cdot \mathrm{grad}_{\vec{p}}\, j_{0,n}(k_\pm r)\right]$$
$$- |\vec{q}|^2 \frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\left[|\vec{p}|\vec{p}\cdot \mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r)\right] + |\vec{p}|^2|\vec{q}|^2 \mathrm{div}_{\vec{p}}\, \mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) =$$
$$= \pm\Bigg\{ \frac{1}{2r^2}\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 j_{0,n-2}(k_\pm r) - (|\vec{p}|^2 + |\vec{q}|^2)\left[2 + \frac{3r}{4}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n}(k_\pm r)$$
$$+ (|\vec{p}|^2 - |\vec{q}|^2)^2 r^2 \left[1 + \frac{2(|\vec{p}|^4 + |\vec{q}|^4) + (|\vec{p}|^2 + |\vec{q}|^2)^2}{2(|\vec{p}|^2 - |\vec{q}|^2)^2}\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\right] \times$$
$$\times \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n+2}(k_\pm r)$$
$$- \frac{(|\vec{p}|^2 + |\vec{q}|^2)(|\vec{p}|^2 - |\vec{q}|^2)^2}{2} r^4 \left[2 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n+4}(k_\pm r)\Bigg\} \qquad \text{(C.27)}$$

Proof.

$$\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\left[|\vec{p}|(\vec{p}\cdot\vec{q}) j_{0,n}(k_\pm r)\right]\right] - |\vec{p}|^2 \frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[|\vec{q}|\vec{q}\cdot \mathrm{grad}_{\vec{p}}\, j_{0,n}(k_\pm r)\right]$$
$$- |\vec{q}|^2 \frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\left[|\vec{p}|\vec{p}\cdot \mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r)\right] + |\vec{p}|^2|\vec{q}|^2 \mathrm{div}_{\vec{p}}\, \mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) =$$
$$= (\vec{p}\cdot\vec{q}) j_{0,n}(k_\pm r) + |\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[(\vec{p}\cdot\vec{q}) j_{0,n}(k_\pm r)\right]$$
$$+ |\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\left[(\vec{p}\cdot\vec{q}) j_{0,n}(k_\pm r)\right] + |\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}|\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\left[(\vec{p}\cdot\vec{q}) j_{0,n}(k_\pm r)\right]$$
$$- |\vec{p}|^2 \vec{q}\cdot \mathrm{grad}_{\vec{p}}\, j_{0,n}(k_\pm r) - |\vec{p}|^2|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[\vec{q}\cdot \mathrm{grad}_{\vec{p}}\, j_{0,n}(k_\pm r)\right]$$
$$- |\vec{q}|^2 \vec{p}\cdot \mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) - |\vec{q}|^2|\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\left[\vec{p}\cdot \mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r)\right]$$
$$+ |\vec{p}|^2|\vec{q}|^2 \mathrm{div}_{\vec{p}}\, \mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) \qquad \text{(C.28)}$$

To proceed, we make use of (C.2b) in order to rewrite the scalar products of gradients with $\vec{p}$ and $\vec{q}$, respectively. Furthermore, by expressing factors $\vec{p}\cdot\vec{q}$ in terms of $k_\pm$ using (C.4) and by inserting (C.3a) for $\mathrm{div}_{\vec{p}}\,\mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r)$ we find

$$\begin{aligned}
\cdots = &\pm\left[\frac{1}{2r^2}j_{0,n-2}(k_\pm r) - \frac{|\vec{p}|^2+|\vec{q}|^2}{2}j_{0,n}(k_\pm r)\right]\\
&\pm|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[\frac{1}{2r^2}j_{0,n-2}(k_\pm r) - \frac{|\vec{p}|^2+|\vec{q}|^2}{2}j_{0,n}(k_\pm r)\right]\\
&\pm|\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\left[\frac{1}{2r^2}j_{0,n-2}(k_\pm r) - \frac{|\vec{p}|^2+|\vec{q}|^2}{2}j_{0,n}(k_\pm r)\right]\\
&\pm|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}|\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\left[\frac{1}{2r^2}j_{0,n-2}(k_\pm r) - \frac{|\vec{p}|^2+|\vec{q}|^2}{2}j_{0,n}(k_\pm r)\right]\\
&\mp|\vec{p}|^2\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r) - (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\right]\\
&\mp|\vec{p}|^2|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r) - (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\right]\\
&\mp|\vec{q}|^2\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r) + (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\right]\\
&\mp|\vec{q}|^2|\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r) + (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\right]\\
&\pm 4|\vec{p}|^2|\vec{q}|^2r^2\left[\frac{3}{2}+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)
\end{aligned}$$

Next, we carry out derivatives with respect to $|\vec{p}|$ and $|\vec{q}|$ which results in

$$\begin{aligned}
\cdots = &\pm\left[\frac{1}{2r^2}j_{0,n-2}(k_\pm r) - \frac{|\vec{p}|^2+|\vec{q}|^2}{2}j_{0,n}(k_\pm r)\right]\\
&\pm\left[\frac{1}{2r^2}|\vec{q}|\frac{\mathrm{d}j_{0,n-2}(k_\pm r)}{\mathrm{d}|\vec{q}|} - |\vec{q}|^2 j_{0,n}(k_\pm r) - \frac{|\vec{p}|^2+|\vec{q}|^2}{2}|\vec{q}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{q}|}\right]\\
&\pm\left[\frac{1}{2r^2}|\vec{p}|\frac{\mathrm{d}j_{0,n-2}(k_\pm r)}{\mathrm{d}|\vec{p}|} - |\vec{p}|^2 j_{0,n}(k_\pm r) - \frac{|\vec{p}|^2+|\vec{q}|^2}{2}|\vec{p}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{p}|}\right]\\
&\pm\left[\frac{1}{2r^2}|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}|\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}j_{0,n-2}(k_\pm r) - |\vec{p}|^2|\vec{q}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{q}|}\right.\\
&\qquad\left. - |\vec{q}|^2|\vec{p}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{p}|} - \frac{|\vec{p}|^2+|\vec{q}|^2}{2}|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}|\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}j_{0,n}(k_\pm r)\right]\\
&\mp|\vec{p}|^2\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r) - (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\right]\\
&\mp|\vec{p}|^2\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}|\vec{q}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{q}|} + 2|\vec{q}|^2r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\right.\\
&\qquad\left. - (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]|\vec{q}|\frac{\mathrm{d}j_{0,n+2}(k_\pm r)}{\mathrm{d}|\vec{q}|}\right]\\
&\mp|\vec{q}|^2\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r) + (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\right]\\
&\mp|\vec{q}|^2\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}|\vec{p}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{p}|} + 2|\vec{p}|^2r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\right.\\
&\qquad\left. + (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]|\vec{p}|\frac{\mathrm{d}j_{0,n+2}(k_\pm r)}{\mathrm{d}|\vec{p}|}\right]\\
&\pm 4|\vec{p}|^2|\vec{q}|^2r^2\left[\frac{3}{2}+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)
\end{aligned}$$

Due to the structural similarity of the derivatives of $j_{0,n}(k_\pm r)$ with respect to $|\vec{p}|$ and $|\vec{q}|$ (see (C.2d)), it is advantageous to group terms such that there are sums and differences of derivatives of $j_{0,n}(k_\pm r)$ with respect to $|\vec{p}|$ and $|\vec{q}|$. In this way, we find

$$\begin{aligned}
\cdots = &\pm\left[\frac{1}{2r^2}j_{0,n-2}(k_\pm r) - 3\frac{|\vec{p}|^2+|\vec{q}|^2}{2}j_{0,n}(k_\pm r)\right]\\
&\pm\frac{1}{2r^2}\left[|\vec{q}|\frac{\mathrm{d}j_{0,n-2}(k_\pm r)}{\mathrm{d}|\vec{q}|} + |\vec{p}|\frac{\mathrm{d}j_{0,n-2}(k_\pm r)}{\mathrm{d}|\vec{p}|}\right]\\
&\mp\frac{|\vec{p}|^2+|\vec{q}|^2}{2}\left[|\vec{q}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{q}|} + |\vec{p}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{p}|}\right]\\
&\pm\frac{1}{2r^2}|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}|\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}j_{0,n-2}(k_\pm r) \mp \frac{|\vec{p}|^2+|\vec{q}|^2}{2}|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}|\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}j_{0,n}(k_\pm r)\\
&\mp\left[(|\vec{p}|^2+|\vec{q}|^2)\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r) - (|\vec{p}|^2-|\vec{q}|^2)^2r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\right]\\
&\mp\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[|\vec{p}|^2|\vec{q}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{q}|} + |\vec{q}|^2|\vec{p}|\frac{\mathrm{d}j_{0,n}(k_\pm r)}{\mathrm{d}|\vec{p}|}\right]\\
&\pm(|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[|\vec{p}|^2|\vec{q}|\frac{\mathrm{d}j_{0,n+2}(k_\pm r)}{\mathrm{d}|\vec{q}|} - |\vec{q}|^2|\vec{p}|\frac{\mathrm{d}j_{0,n+2}(k_\pm r)}{\mathrm{d}|\vec{p}|}\right]\\
&\pm 4|\vec{p}|^2|\vec{q}|^2r^2\left[\frac{1}{2}+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)
\end{aligned}$$

Now we make use of the explicit formulas (C.2d) and (C.3c) which turn the expression into the following form

$$\begin{aligned}
\cdots = &\pm\left[\frac{1}{2r^2}j_{0,n-2}(k_\pm r) - 3\frac{|\vec{p}|^2+|\vec{q}|^2}{2}j_{0,n}(k_\pm r)\right]\\
&\pm\frac{1}{2r^2}\left[r\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n-2}(k_\pm r) \mp \frac{|\vec{p}|^2+|\vec{q}|^2}{2}\left[r\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n}(k_\pm r)\\
&\pm\frac{1}{2r^2}\Bigg[\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 j_{0,n-2}(k_\pm r) - (|\vec{p}|^2+|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n}(k_\pm r)\\
&\qquad - (|\vec{p}|^2-|\vec{q}|^2)^2r^4\left[2+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\Bigg]\\
&\mp\frac{|\vec{p}|^2+|\vec{q}|^2}{2}\Bigg[\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 j_{0,n}(k_\pm r) - (|\vec{p}|^2+|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\\
&\qquad - (|\vec{p}|^2-|\vec{q}|^2)^2r^4\left[2+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+4}(k_\pm r)\Bigg]\\
&\mp\left[(|\vec{p}|^2+|\vec{q}|^2)\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r) - (|\vec{p}|^2-|\vec{q}|^2)^2r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\right]\\
&\mp\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[(|\vec{p}|^2+|\vec{q}|^2)\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n}(k_\pm r) - (|\vec{p}|^2-|\vec{q}|^2)^2r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)\right]\\
&\pm(|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\Bigg[(|\vec{p}|^2-|\vec{q}|^2)\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,n+2}(k_\pm r)\\
&\qquad - r^2(|\vec{p}|^4-|\vec{q}|^4)\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+4}(k_\pm r)\Bigg]\\
&\pm 4|\vec{p}|^2|\vec{q}|^2r^2\left[\frac{1}{2}+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,n+2}(k_\pm r)
\end{aligned}$$

By sorting and grouping terms according to their indices we finally end up with

$$\begin{aligned}\cdots = \pm\Bigg\{ &\frac{1}{2r^2}\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 j_{0,n-2}(k_\pm r) - (|\vec{p}|^2+|\vec{q}|^2)\left[2+\frac{3r}{4}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n}(k_\pm r)\\ &+ (|\vec{p}|^2-|\vec{q}|^2)^2 r^2\left[1+\frac{2(|\vec{p}|^4+|\vec{q}|^4)+(|\vec{p}|^2+|\vec{q}|^2)^2}{2(|\vec{p}|^2-|\vec{q}|^2)^2}\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\right]\times\\ &\times\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n+2}(k_\pm r)\\ &- \frac{(|\vec{p}|^2+|\vec{q}|^2)(|\vec{p}|^2-|\vec{q}|^2)^2}{2} r^4\left[2+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,n+4}(k_\pm r)\Bigg\} \qquad \text{(C.29)}\end{aligned}$$

This concludes the proof. □

Auxiliary Calculation C.1.8 (Integrand of $\vec{\Phi}_{lm}\cdot\vec{\Phi}_{l'm'}$ in (C.58) in Lemma C.4.1)

$$\begin{aligned}&\mathrm{div}_{\vec{p}}\left[h(|\vec{p}|)\,\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)(\vec{p}\cdot\vec{q})j_{0,1}(k_\pm r)\right)\right] - \vec{q}\cdot\mathrm{grad}_{\vec{p}}\left[h(|\vec{p}|)\left(\vec{p}\cdot\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\right)\right)\right]\\ &\quad= h'(|\vec{p}|)|\vec{p}|k(|\vec{q}|)j_{0,1}(k_\pm r)\\ &\quad\quad+ h(|\vec{p}|)k(|\vec{q}|)\left[\left[3+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,1}(k_\pm r) + (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,3}(k_\pm r)\right] \qquad \text{(C.30)}\end{aligned}$$

Proof.

$$\begin{aligned}&\mathrm{div}_{\vec{p}}\left[h(|\vec{p}|)\,\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)(\vec{p}\cdot\vec{q})j_{0,1}(k_\pm r)\right)\right] - \vec{q}\cdot\mathrm{grad}_{\vec{p}}\left[h(|\vec{p}|)\left(\vec{p}\cdot\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\right)\right)\right] =\\ &= \frac{h'(|\vec{p}|)}{|\vec{p}|}\vec{p}\cdot\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)(\vec{p}\cdot\vec{q})j_{0,1}(k_\pm r)\right) + h(|\vec{p}|)\mathrm{div}_{\vec{p}}\,\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)(\vec{p}\cdot\vec{q})j_{0,1}(k_\pm r)\right)\\ &\quad- \frac{h'(|\vec{p}|)}{|\vec{p}|}(\vec{q}\cdot\vec{p})\left(\vec{p}\cdot\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\right)\right) - h(|\vec{p}|)\vec{q}\cdot\mathrm{grad}_{\vec{p}}\left(\vec{p}\cdot\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\right)\right)\end{aligned}$$

Combining the first and third term as well as the second and fourth one we find

$$\begin{aligned}\cdots = &\frac{h'(|\vec{p}|)}{|\vec{p}|}\left[\vec{p}\cdot\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)(\vec{p}\cdot\vec{q})j_{0,1}(k_\pm r)\right) - (\vec{q}\cdot\vec{p})\left(\vec{p}\cdot\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\right)\right)\right]\\ &+ h(|\vec{p}|)\Big[\mathrm{div}_{\vec{p}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\vec{p} + (\vec{p}\cdot\vec{q})\,\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\right)\right)\\ &\qquad - \vec{q}\cdot\left(\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\right) + \vec{p}\,\mathrm{div}_{\vec{p}}\,\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\right)\right)\Big]\end{aligned}$$

Simplifying term proportional to $h'(|\vec{p}|)$ and expanding the term proportional to $h(|\vec{p}|)$ yields

$$\begin{aligned}&= \frac{h'(|\vec{p}|)}{|\vec{p}|}\left[k(|\vec{q}|)j_{0,1}(k_\pm r)\vec{p}\cdot\mathrm{grad}_{\vec{q}}(\vec{p}\cdot\vec{q})\right]\\ &\quad+ h(|\vec{p}|)\Big[\mathrm{div}_{\vec{p}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\vec{p}\right) + \left(\mathrm{grad}_{\vec{p}}(\vec{p}\cdot\vec{q})\right)\cdot\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\right)\\ &\qquad+ (\vec{p}\cdot\vec{q})\mathrm{div}_{\vec{p}}\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\right)\\ &\qquad\quad- \vec{q}\cdot\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\right) - (\vec{p}\cdot\vec{q})\mathrm{div}_{\vec{p}}\,\mathrm{grad}_{\vec{q}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\right)\Big]\end{aligned}$$

By using $\mathrm{grad}_{\vec{p}}(\vec{p}\cdot\vec{q}) = \vec{q}$ and $\mathrm{grad}_{\vec{q}}(\vec{p}\cdot\vec{q}) = \vec{p}$ and cancelling terms, the expression reduces to

$$\cdots = h'(|\vec{p}|)|\vec{p}|k(|\vec{q}|)j_{0,1}(k_\pm r) + h(|\vec{p}|)\mathrm{div}_{\vec{p}}\left(k(|\vec{q}|)j_{0,1}(k_\pm r)\vec{p}\right)$$

Pulling $k(|\vec{q}|)$ outside the second term, computing the divergence and using (C.2a), we finally end up with

$$\begin{aligned}\cdots &= h'(|\vec{p}|)|\vec{p}|k(|\vec{q}|)j_{0,1}(k_\pm r) + h(|\vec{p}|)k(|\vec{q}|)\Big(3j_{0,n}(k_\pm r) + \vec{p}\cdot \mathrm{grad}_{\vec{p}}\, j_{0,1}(k_\pm r)\Big)\\ &\overset{(C.2a)}{=} h'(|\vec{p}|)|\vec{p}|k(|\vec{q}|)j_{0,1}(k_\pm r)\\ &\quad + h(|\vec{p}|)k(|\vec{q}|)\left[\left[3+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,1}(k_\pm r) + (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,3}(k_\pm r)\right] \end{aligned} \tag{C.31}$$

This concludes the proof. □

C.2 Evaluation of Dotted Terms

The computation of the position space angular integrals (4.27a) and (4.27b) in Proposition 4.2.4 (Position Space Angular Integration of Υ_{lm}, $\Upsilon_{lm|l'm'}$, $\overset{*}{\Upsilon}_{lm|l'm'}$) requires to evaluate the integrals

$$\int_{S^2} \mathrm{d}\Omega_\xi\; \vec{\xi}\cdot \vec{\mathbf{Y}}_{lm}(\theta_p,\varphi_p)\mathrm{e}^{-\mathrm{i}\vec{p}\cdot\vec{\xi}} \qquad \text{where} \qquad \vec{\mathbf{Y}}_{lm}\in\{\vec{Y}_{lm},\vec{\Psi}_{lm},\vec{\Phi}_{lm}\}$$

appearing in the entries of the integral of Υ_{lm} as well as the integrals

$$\int_{S^2} \mathrm{d}\Omega_\xi\; \vec{\xi}\cdot \vec{\mathbf{Y}}_{lm}(\theta_p,\varphi_p)\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} \qquad \text{and} \qquad \int_{S^2} \mathrm{d}\Omega_\xi\; \vec{\xi}\cdot \vec{\mathbf{Y}}_{l'm'}(\theta_q,\varphi_q)\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}}$$

which correspond to the *dotted-unprimed* and *dotted-primed* terms of $\Upsilon_{lm|l'm'}$, respectively. All these integrals can be computed systematically using the following lemma.

Lemma C.2.1 (Angular Integration of Dotted Terms)

For any functions $h,k\in C^1(\mathbb{R}_0^+,\mathbb{R})$ and for $\vec{\mathbf{Y}}_{l^{(\prime)}m^{(\prime)}}\in\{\vec{Y}_{l^{(\prime)}m^{(\prime)}},\vec{\Phi}_{l^{(\prime)}m^{(\prime)}},\vec{\Psi}_{l^{(\prime)}m^{(\prime)}}\}$ the relation

$$\begin{aligned}&\int_{\mathbb{R}^3}\mathrm{d}^3\vec{p}\; h(|\vec{p}|)\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\; k(|\vec{q}|)\int_{S^2}\mathrm{d}\Omega_\xi \begin{Bmatrix}\vec{\xi}\cdot\vec{\mathbf{Y}}_{lm}(\theta_p,\varphi_p)\\ \vec{\xi}\cdot\vec{\mathbf{Y}}_{l'm'}(\theta_q,\varphi_q)\end{Bmatrix}\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} =\\ &= 4\pi\mathrm{i}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{p}\; h(|\vec{p}|)\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\; k(|\vec{q}|)\sum_{n=1}^{5}\left\{\begin{matrix}\frac{Y_{lm}}{|\vec{p}|}\begin{Bmatrix}\dot{\mathfrak{m}}^{(n)}_{\vec{\mathbf{Y}}}\, j_{0,n}(k_+r)\\ \dot{\mathfrak{n}}^{(n)}_{\vec{\mathbf{Y}}}\, j_{0,n}(k_-r)\end{Bmatrix}\\ \frac{Y_{l'm'}}{|\vec{q}|}\begin{Bmatrix}\acute{\dot{\mathfrak{m}}}^{(n)}_{\vec{\mathbf{Y}}'}\, j_{0,n}(k_+r)\\ \acute{\dot{\mathfrak{n}}}^{(n)}_{\vec{\mathbf{Y}}'}\, j_{0,n}(k_-r)\end{Bmatrix}\end{matrix}\right\}\end{aligned} \tag{C.32}$$

holds, where the differential operators $\dot{\mathfrak{m}}^{(n)}_{\vec{\mathbf{Y}}}$, $\dot{\mathfrak{n}}^{(n)}_{\vec{\mathbf{Y}}}$, $\acute{\dot{\mathfrak{m}}}^{(n)}_{\vec{\mathbf{Y}}'}$ and $\acute{\dot{\mathfrak{n}}}^{(n)}_{\vec{\mathbf{Y}}'}$ with respect to r are entries of operator-valued, dimensionless (3×1)-matrices $\dot{\mathfrak{m}}^{(n)}$, $\dot{\mathfrak{n}}^{(n)}$, $\acute{\dot{\mathfrak{m}}}^{(n)}$ and $\acute{\dot{\mathfrak{n}}}^{(n)}$ which are explicitly given by

$$\begin{Bmatrix}\dot{\mathfrak{m}}^{(1)}\\ \dot{\mathfrak{n}}^{(1)}\end{Bmatrix} = \begin{pmatrix}1\\ [1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}]\\ 0\end{pmatrix}\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.32a}$$

$$\begin{Bmatrix} \dot{\mathfrak{m}}^{(3)} \\ \dot{\mathfrak{n}}^{(3)} \end{Bmatrix} = \begin{pmatrix} (|\vec{p}|^2 - |\vec{q}|^2)r^2 \\ -2(|\vec{p}|^2 + |\vec{q}|^2)r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \\ 0 \end{pmatrix} \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.32b}$$

$$\begin{Bmatrix} \dot{\mathfrak{m}}^{(5)} \\ \dot{\mathfrak{n}}^{(5)} \end{Bmatrix} = (|\vec{p}|^2 - |\vec{q}|^2)^2 r^4 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \left[2 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.32c}$$

$$\begin{Bmatrix} \ddot{\mathfrak{m}}^{(1)} \\ \ddot{\mathfrak{n}}^{(1)} \end{Bmatrix} = \begin{Bmatrix} +1 \\ -1 \end{Bmatrix} \begin{pmatrix} 1 \\ \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \\ 0 \end{pmatrix} \left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.32d}$$

$$\begin{Bmatrix} \ddot{\mathfrak{m}}^{(3)} \\ \ddot{\mathfrak{n}}^{(3)} \end{Bmatrix} = \begin{Bmatrix} -1 \\ +1 \end{Bmatrix} \begin{pmatrix} (|\vec{p}|^2 - |\vec{q}|^2)r^2 \\ 2(|\vec{p}|^2 + |\vec{q}|^2)r^2\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \\ 0 \end{pmatrix} \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.32e}$$

$$\begin{Bmatrix} \ddot{\mathfrak{m}}^{(5)} \\ \ddot{\mathfrak{n}}^{(5)} \end{Bmatrix} = \begin{Bmatrix} +1 \\ -1 \end{Bmatrix} (|\vec{p}|^2 - |\vec{q}|^2)^2 r^4 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \left[2 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.32f}$$

Proof. We start by rewriting the scalar products $\vec{\xi}\cdot\vec{\mathbf{Y}}_{lm}(\theta_p,\varphi_p)$ and $\vec{\xi}\cdot\vec{\mathbf{Y}}_{l'm'}(\theta_q,\varphi_q)$ as gradients of the exponential factor with respect to $\vec{p}$ and $\vec{q}$, respectively, and subsequently compute the angular integral in position space using Proposition C.1.1. In this way, we obtain

$$\begin{aligned}
&\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \int_{S^2} \mathrm{d}\Omega_\xi \begin{Bmatrix} \vec{\xi}\cdot\vec{\mathbf{Y}}_{lm}(\theta_p,\varphi_p) \\ \vec{\xi}\cdot\vec{\mathbf{Y}}_{l'm'}(\theta_q,\varphi_q) \end{Bmatrix} \mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} = \\
&\quad = \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \int_{S^2} \mathrm{d}\Omega_\xi \begin{Bmatrix} \mathrm{i}\vec{\mathbf{Y}}_{lm}(\theta_p,\varphi_p)\cdot\mathrm{grad}_{\vec{p}} \\ \pm\mathrm{i}\vec{\mathbf{Y}}_{l'm'}(\theta_q,\varphi_q)\cdot\mathrm{grad}_{\vec{q}} \end{Bmatrix} \mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} \\
&\quad \overset{(C.1)}{=} 4\pi\mathrm{i} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \begin{Bmatrix} \vec{\mathbf{Y}}_{lm}(\theta_p,\varphi_p)\cdot\mathrm{grad}_{\vec{p}} \\ \pm\vec{\mathbf{Y}}_{l'm'}(\theta_q,\varphi_q)\cdot\mathrm{grad}_{\vec{q}} \end{Bmatrix} j_{0,1}(k_\pm r)
\end{aligned}$$

Computing the gradients of $j_{0,1}(k_\pm r)$ with respect to $\vec{p}$ and $\vec{q}$ using (C.2a) and (C.2a), respectively, turns the expression into the form

$$\ldots \underset{(C.2a)}{\overset{(C.2a)}{=}} 8\pi\mathrm{i} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \begin{Bmatrix} \vec{\mathbf{Y}}_{lm}(\theta_p,\varphi_p)\cdot(\vec{p}\pm\vec{q}) \\ \vec{\mathbf{Y}}_{l'm'}(\theta_q,\varphi_q)\cdot(\vec{p}\pm\vec{q}) \end{Bmatrix} r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,3}(k_\pm r) \tag{C.33}$$

To proceed, we have to consider the three possible choices for $\vec{\mathbf{Y}}_{l^{(\prime)}m^{(\prime)}}$ separately.

(1) $\vec{\mathbf{Y}}_{lm} = \vec{Y}_{lm}$

In the first case, namely for the *radial* spherical harmonic $\vec{\mathbf{Y}}_{l^{(\prime)}m^{(\prime)}} = \vec{Y}_{l^{(\prime)}m^{(\prime)}}$, we insert the definitions $\vec{Y}_{lm} \overset{(4.4a)}{=} \frac{\vec{p}}{|\vec{p}|}Y_{lm}$ and $\vec{Y}_{l'm'} \overset{(4.4a)}{=} \frac{\vec{q}}{|\vec{q}|}Y_{l'm'}$ into (C.33), make use of the relations (C.4a), (C.4b) and thus obtain

$$\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|) \int_{S^2} \mathrm{d}\Omega_\xi \begin{Bmatrix} \vec{\xi}\cdot\vec{Y}_{lm}(\theta_p,\varphi_p) \\ \vec{\xi}\cdot\vec{Y}_{l'm'}(\theta_q,\varphi_q) \end{Bmatrix} \mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} =$$

$$\overset{(C.33)}{\underset{(C.4)}{=}} 4\pi\mathrm{i} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|) r^2 \left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \begin{Bmatrix} \frac{Y_{lm}}{|\vec{p}|}\Big[r^{-2}j_{0,1}(k_\pm r) \\ \qquad +(|\vec{p}|^2-|\vec{q}|^2)j_{0,3}(k_\pm r)\Big] \\ \pm\frac{Y_{l'm'}}{|\vec{q}|}\Big[r^{-2}j_{0,1}(k_\pm r) \\ \qquad -(|\vec{p}|^2-|\vec{q}|^2)j_{0,3}(k_\pm r)\Big] \end{Bmatrix}$$

$$= 4\pi\mathrm{i} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|) \begin{Bmatrix} \frac{Y_{lm}}{|\vec{p}|}\Big[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,1}(k_\pm r) \\ \qquad +(|\vec{p}|^2-|\vec{q}|^2)r^2\big[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\big]j_{0,3}(k_\pm r)\Big] \\ \pm\frac{Y_{l'm'}}{|\vec{q}|}\Big[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}j_{0,1}(k_\pm r) \\ \qquad -(|\vec{p}|^2-|\vec{q}|^2)r^2\big[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\big]j_{0,3}(k_\pm r)\Big] \end{Bmatrix}$$

$$= 4\pi\mathrm{i} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|) \sum_{n=1}^{3} \begin{Bmatrix} \frac{Y_{lm}}{|\vec{p}|}\begin{Bmatrix} \dot{\mathfrak{m}}^{(n)}_{\vec{Y}} j_{0,n}(k_+ r) \\ \dot{\mathfrak{n}}^{(n)}_{\vec{Y}} j_{0,n}(k_- r) \end{Bmatrix} \\ \frac{Y_{l'm'}}{|\vec{q}|}\begin{Bmatrix} \acute{\dot{\mathfrak{m}}}^{(n)}_{\vec{Y}'} j_{0,n}(k_+ r) \\ \acute{\dot{\mathfrak{n}}}^{(n)}_{\vec{Y}'} j_{0,n}(k_- r) \end{Bmatrix} \end{Bmatrix} \tag{C.34}$$

Here $\dot{\mathfrak{m}}^{(n)}_{\vec{Y}}$, $\dot{\mathfrak{n}}^{(n)}_{\vec{Y}}$ and $\acute{\dot{\mathfrak{m}}}^{(n)}_{\vec{Y}'}$, $\acute{\dot{\mathfrak{n}}}^{(n)}_{\vec{Y}'}$ are differential operators with respect to r, explicitly given by

$$\begin{Bmatrix} \dot{\mathfrak{m}}^{(1)}_{\vec{Y}} \\ \dot{\mathfrak{n}}^{(1)}_{\vec{Y}} \end{Bmatrix} = \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} \tag{C.35a}$$

$$\begin{Bmatrix} \dot{\mathfrak{m}}^{(3)}_{\vec{Y}} \\ \dot{\mathfrak{n}}^{(3)}_{\vec{Y}} \end{Bmatrix} = (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.35b}$$

$$\begin{Bmatrix} \acute{\dot{\mathfrak{m}}}^{(1)}_{\vec{Y}'} \\ \acute{\dot{\mathfrak{n}}}^{(1)}_{\vec{Y}'} \end{Bmatrix} = \begin{Bmatrix} +1 \\ -1 \end{Bmatrix} \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} \tag{C.35c}$$

$$\begin{Bmatrix} \acute{\dot{\mathfrak{m}}}^{(3)}_{\vec{Y}'} \\ \acute{\dot{\mathfrak{n}}}^{(3)}_{\vec{Y}'} \end{Bmatrix} = \begin{Bmatrix} -1 \\ +1 \end{Bmatrix} (|\vec{p}|^2-|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.35d}$$

Here we have implicitly chosen the convention that operators $\mathfrak{m}$ always act on $j_{0,n}(k_+ r)$ while operators $\mathfrak{n}$ act on $j_{0,n}(k_- r)$. Additionally, dotted-unprimed terms always come with Y_{lm} while dotted-primed terms come with $Y_{l'm'}$.

(2) $\vec{\mathbf{Y}}_{lm} = \vec{\Psi}_{lm}$

In the second case, namely for the *first tangential* vector spherical harmonic $\vec{\mathbf{Y}}_{l^{(\prime)}m^{(\prime)}} = \vec{\Psi}_{l^{(\prime)}m^{(\prime)}}$, we again insert the definitions $\vec{\Psi}_{lm} \overset{(4.4b)}{=} |\vec{p}|\,\mathrm{grad}_{\vec{p}}\,Y_{lm}$ and $\vec{\Psi}_{l'm'} \overset{(4.4b)}{=} |\vec{q}|\,\mathrm{grad}_{\vec{q}}\,Y_{l'm'}$ into (C.33) and make use of the fact that the parts $\vec{p}\cdot\vec{\Psi}_{lm}$ and $\vec{q}\cdot\vec{\Psi}_{l'm'}$ vanish for reasons of orthogonality. We are thus left with

$$\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|) \int_{S^2} \mathrm{d}\Omega_\xi \begin{Bmatrix} \vec{\xi}\cdot\vec{\Psi}_{lm}(\theta_p,\varphi_p) \\ \vec{\xi}\cdot\vec{\Psi}_{l'm'}(\theta_q,\varphi_q) \end{Bmatrix} \mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} =$$

$$\overset{(C.33)}{=} 8\pi\mathrm{i} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|) \begin{Bmatrix} \pm|\vec{p}|\,\mathrm{grad}_{\vec{p}}\,Y_{lm}\cdot\vec{q} \\ |\vec{q}|\,\mathrm{grad}_{\vec{q}}\,Y_{l'm'}\cdot\vec{p} \end{Bmatrix} r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,3}(k_\pm r)$$

To get rid of the derivatives of spherical harmonics, we integrate by parts with respect to $\vec{p}$ and $\vec{q}$, respectively, which results in

$$\cdots = 8\pi \mathrm{i} r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q} \begin{Bmatrix} \pm k(|\vec{q}|)\Big[\mathrm{div}_{\vec{p}}\big(h(|\vec{p}|)|\vec{p}|Y_{lm} j_{0,3}(k_\pm r)\vec{q}\big) \\ \qquad -Y_{lm}\mathrm{div}_{\vec{p}}\big(h(|\vec{p}|)|\vec{p}|j_{0,3}(k_\pm r)\vec{q}\big)\Big] \\ h(|\vec{p}|)\Big[\mathrm{div}_{\vec{q}}\big(k(|\vec{q}|)|\vec{q}|Y_{l'm'} j_{0,3}(k_\pm r)\vec{p}\big) \\ \qquad -Y_{l'm'}\mathrm{div}_{\vec{q}}\big(k(|\vec{q}|)|\vec{q}|j_{0,3}(k_\pm r)\vec{p}\big)\Big] \end{Bmatrix}$$

Making use of the divergence theorem to rewrite the first term in both cases, and carrying out the derivative in the second term results in

$$\cdots = 8\pi \mathrm{i} r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \begin{Bmatrix} \pm \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \lim\limits_{|\vec{p}|\to\infty} \Big[h(|\vec{p}|)|\vec{p}|^2 \int\limits_{S^2} \mathrm{d}\Omega_p\; Y_{lm} j_{0,3}(k_\pm r)(\vec{p}\cdot\vec{q})\Big] \\ \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \lim\limits_{|\vec{q}|\to\infty} \Big[k(|\vec{q}|)|\vec{q}|^2 \int\limits_{S^2} \mathrm{d}\Omega_q\; Y_{l'm'} j_{0,3}(k_\pm r)(\vec{p}\cdot\vec{q})\Big] \end{Bmatrix}$$

$$- 8\pi \mathrm{i} r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q} \begin{Bmatrix} \pm k(|\vec{q}|)Y_{lm}\cdot\Big[\frac{(h(|\vec{p}|)|\vec{p}|)'}{|\vec{p}|}(\vec{p}\cdot\vec{q})j_{0,3}(k_\pm r) \\ \qquad + h(|\vec{p}|)|\vec{p}|\vec{q}\cdot\mathrm{grad}_{\vec{p}}\, j_{0,3}(k_\pm r)\Big] \\ h(|\vec{p}|)Y_{l'm'}\Big[\frac{(k(|\vec{q}|)|\vec{q}|)'}{|\vec{q}|}(\vec{p}\cdot\vec{q})j_{0,3}(k_\pm r) \\ \qquad + k(|\vec{q}|)|\vec{q}|\vec{p}\cdot\mathrm{grad}_{\vec{q}}\, j_{0,3}(k_\pm r)\Big] \end{Bmatrix}$$

Integrating the terms which contain derivatives of $h(|\vec{p}|)$ and $k(|\vec{q}|)$ with respect to $|\vec{p}|$ and $|\vec{q}|$, respectively, and taking into account that the boundary terms at $|\vec{p}| = 0$ and $|\vec{q}| = 0$ vanish as $h, k \in C^1(\mathbb{R}_0^+, \mathbb{R})$, we find

$$\cdots = 8\pi \mathrm{i} r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \begin{Bmatrix} \pm \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \lim\limits_{|\vec{p}|\to\infty} \Big[h(|\vec{p}|)|\vec{p}|^2 \int\limits_{S^2} \mathrm{d}\Omega_p\; Y_{lm} j_{0,3}(k_\pm r)(\vec{p}\cdot\vec{q})\Big] \\ \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \lim\limits_{|\vec{q}|\to\infty} \Big[k(|\vec{q}|)|\vec{q}|^2 \int\limits_{S^2} \mathrm{d}\Omega_q\; Y_{l'm'} j_{0,3}(k_\pm r)(\vec{p}\cdot\vec{q})\Big] \end{Bmatrix}$$

$$- 8\pi \mathrm{i} r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \begin{Bmatrix} \pm \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \lim\limits_{|\vec{p}|\to\infty} \Big[h(|\vec{p}|)|\vec{p}|^2 \int\limits_{S^2} \mathrm{d}\Omega_p\; Y_{lm}(\vec{p}\cdot\vec{q}) j_{0,3}(k_\pm r)\Big] \\ \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \lim\limits_{|\vec{q}|\to\infty} \Big[k(|\vec{q}|)|\vec{q}|^2 \int\limits_{S^2} \mathrm{d}\Omega_q\; Y_{l'm'}(\vec{p}\cdot\vec{q}) j_{0,3}(k_\pm r)\Big] \end{Bmatrix}$$

$$- 8\pi \mathrm{i} r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \begin{Bmatrix} \pm \frac{Y_{lm}}{|\vec{p}|}\Big[-\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\big[|\vec{p}|\vec{p}\cdot\vec{q}\, j_{0,3}(k_\pm r)\big] \\ \qquad + |\vec{p}|^2\vec{q}\cdot\mathrm{grad}_{\vec{p}}\, j_{0,3}(k_\pm r)\Big] \\ \frac{Y_{l'm'}}{|\vec{q}|}\Big[-\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\big[|\vec{q}|\vec{p}\cdot\vec{q}\, j_{0,3}(k_\pm r)\big] \\ \qquad + |\vec{q}|^2\vec{p}\cdot\mathrm{grad}_{\vec{q}}\, j_{0,3}(k_\pm r)\Big] \end{Bmatrix}$$

Cancelling the first term against the second and making use of Auxiliary Calculation C.1.4 we finally arrive at

$$\ldots \overset{\text{(C.21)}}{=} 4\pi \mathrm{i} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \sum_{n=1}^{5} \begin{Bmatrix} \frac{Y_{lm}}{|\vec{p}|}\begin{cases} \dot{\mathfrak{m}}^{(n)}_{\vec{\Psi}}\, j_{0,n}(k_+ r) \\ \dot{\mathfrak{n}}^{(n)}_{\vec{\Psi}}\, j_{0,n}(k_- r) \end{cases} \\ \frac{Y_{l'm'}}{|\vec{q}|}\begin{cases} \dot{\mathfrak{m}}'^{(n)}_{\vec{\Psi}'}\, j_{0,n}(k_+ r) \\ \dot{\mathfrak{n}}'^{(n)}_{\vec{\Psi}'}\, j_{0,n}(k_- r) \end{cases} \end{Bmatrix} \tag{C.36}$$

where

$$\begin{Bmatrix} \dot{\mathfrak{m}}^{(1)}_{\vec{\Psi}} \\ \dot{\mathfrak{n}}^{(1)}_{\vec{\Psi}} \end{Bmatrix} = \left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.37a}$$

$$\begin{Bmatrix} \dot{\mathfrak{m}}^{(3)}_{\vec{\Psi}} \\ \dot{\mathfrak{n}}^{(3)}_{\vec{\Psi}} \end{Bmatrix} = -2(|\vec{p}|^2+|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 \tag{C.37b}$$

$$\begin{Bmatrix} \dot{\mathfrak{m}}^{(5)}_{\vec{\Psi}} \\ \dot{\mathfrak{n}}^{(5)}_{\vec{\Psi}} \end{Bmatrix} = (|\vec{p}|^2-|\vec{q}|^2)^2r^4\left[2+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.37c}$$

$$\begin{Bmatrix} \ddot{\mathfrak{m}}^{(1)}_{\vec{\Psi}'} \\ \ddot{\mathfrak{n}}^{(1)}_{\vec{\Psi}'} \end{Bmatrix} = \begin{Bmatrix} +1 \\ -1 \end{Bmatrix}\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.37d}$$

$$\begin{Bmatrix} \ddot{\mathfrak{m}}^{(3)}_{\vec{\Psi}'} \\ \ddot{\mathfrak{n}}^{(3)}_{\vec{\Psi}'} \end{Bmatrix} = \begin{Bmatrix} -1 \\ +1 \end{Bmatrix} 2(|\vec{p}|^2+|\vec{q}|^2)r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 \tag{C.37e}$$

$$\begin{Bmatrix} \ddot{\mathfrak{m}}^{(5)}_{\vec{\Psi}'} \\ \ddot{\mathfrak{n}}^{(5)}_{\vec{\Psi}'} \end{Bmatrix} = \begin{Bmatrix} +1 \\ -1 \end{Bmatrix}(|\vec{p}|^2-|\vec{q}|^2)^2r^4\left[2+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.37f}$$

(3) $\vec{\mathbf{Y}}_{lm} = \vec{\Phi}_{lm}$

In the third case, namely for the *second tangential* vector spherical harmonic $\vec{\mathbf{Y}}_{l^{(\prime)}m^{(\prime)}} = \vec{\Phi}_{l^{(\prime)}m^{(\prime)}}$, we once more insert the definitions $\vec{\Psi}_{lm} = \vec{p}\times\mathrm{grad}_{\vec{p}}Y_{lm}$ and $\vec{\Psi}_{l'm'} = \vec{q}\times\mathrm{grad}_{\vec{q}}Y_{l'm'}$ into (C.33) and make use of the fact that the parts $\vec{p}\cdot\vec{\Psi}_{lm}$ and $\vec{q}\cdot\vec{\Psi}_{l'm'}$ vanish for orthogonality reasons. We are thus left with

$$\int_{\mathbb{R}^3}\mathrm{d}^3\vec{p}\;h(|\vec{p}|)\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\;k(|\vec{q}|)\int_{S^2}\mathrm{d}\Omega_\xi\;\begin{Bmatrix}\vec{\xi}\cdot\vec{\Phi}_{lm}(\theta_p,\varphi_p)\\ \vec{\xi}\cdot\vec{\Phi}_{l'm'}(\theta_q,\varphi_q)\end{Bmatrix}\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} =$$

$$\overset{\text{(C.33)}}{=} 8\pi\mathrm{i}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{p}\;h(|\vec{p}|)\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\;k(|\vec{q}|)\begin{Bmatrix}\pm\big(\vec{p}\times\mathrm{grad}_{\vec{p}}Y_{lm}\big)\cdot\vec{q}\\ \big(\vec{q}\times\mathrm{grad}_{\vec{q}}Y_{l'm'}\big)\cdot\vec{p}\end{Bmatrix}r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,3}(k_\pm r)$$

To get rid of the derivatives of spherical harmonics, we exploit the cyclicity of the triple product and subsequently integrate by parts with respect to $\vec{p}$ and $\vec{q}$, respectively, which leaves us with

$$\cdots = 8\pi\mathrm{i}r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\int_{\mathbb{R}^3}\mathrm{d}^3\vec{p}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\begin{Bmatrix}\pm k(|\vec{q}|)\Big[\mathrm{div}_{\vec{p}}\big(h(|\vec{p}|)Y_{lm}j_{0,3}(k_\pm r)(\vec{q}\times\vec{p})\big) \\ \qquad -Y_{lm}\mathrm{div}_{\vec{p}}\big(h(|\vec{p}|)j_{0,3}(k_\pm r)(\vec{q}\times\vec{p})\big)\Big] \\ h(|\vec{p}|)\Big[\mathrm{div}_{\vec{q}}\big(k(|\vec{q}|)Y_{l'm'}j_{0,3}(k_\pm r)(\vec{p}\times\vec{q})\big) \\ \qquad -Y_{l'm'}\mathrm{div}_{\vec{q}}\big(k(|\vec{q}|)j_{0,3}(k_\pm r)(\vec{p}\times\vec{q})\big)\Big]\end{Bmatrix}$$

Making use of the divergence theorem to rewrite the first term in both cases and carrying out the derivative in the second term results in

$$\cdots = 8\pi\mathrm{i}r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\begin{Bmatrix}\pm\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\;k(|\vec{q}|)\lim_{|\vec{p}|\to\infty}\Big[h(|\vec{p}|)|\vec{p}|^2\int_{S^2}\mathrm{d}\Omega_p\;Y_{lm}j_{0,3}(k_\pm r)(\vec{q}\times\vec{p})\cdot\vec{p}\Big]\\ \int_{\mathbb{R}^3}\mathrm{d}^3\vec{p}\;h(|\vec{p}|)\lim_{|\vec{q}|\to\infty}\Big[k(|\vec{q}|)|\vec{q}|^2\int_{S^2}\mathrm{d}\Omega_q\;Y_{l'm'}j_{0,3}(k_\pm r)(\vec{p}\times\vec{q})\cdot\vec{q}\Big]\end{Bmatrix}$$

$$
- 8\pi \mathrm{i} r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q} \begin{Bmatrix} \pm Y_{lm} \cdot \Big[\frac{h'(|\vec{p}\,|)}{|\vec{p}\,|}\vec{p} \cdot (\vec{q} \times \vec{p}\,) j_{0,3}(k_\pm r) \\ \quad + h(|\vec{p}\,|) j_{0,3}(k_\pm r) \mathrm{div}_{\vec{p}}(\vec{q} \times \vec{p}\,) \\ \quad + h(|\vec{p}\,|)(\vec{q} \times \vec{p}\,) \cdot \mathrm{grad}_{\vec{p}}\, j_{0,3}(k_\pm r)\Big] \\ Y_{l'm'} \Big[\frac{k'(|\vec{q}\,|)}{|\vec{q}\,|}\vec{q} \cdot (\vec{p} \times \vec{q}\,) j_{0,3}(k_\pm r) \\ \quad + k(|\vec{q}\,|) j_{0,3}(k_\pm r) \mathrm{div}_{\vec{q}}(\vec{p} \times \vec{q}\,) \\ \quad + k(|\vec{q}\,|)(\vec{p} \times \vec{q}\,) \cdot \mathrm{grad}_{\vec{q}}\, j_{0,3}(k_\pm r)\Big] \end{Bmatrix} \tag{C.38}
$$

In this expression the boundary terms as well as the terms containing derivatives $h'(|\vec{p}\,|)$ an $k'(|\vec{q}\,|)$ vanish by exploiting the cyclicity of the triple product and the properties of the cross product. Recalling that according to (C.2a) and (C.2a) the gradients of $j_{0,3}(k_\pm r)$ with respect to $\vec{p}$ and $\vec{q}$ are both proportional to $(\vec{p} \pm \vec{q}\,)$, also these terms vanish by the same reasoning. Finally, the terms containing divergences also vanish due to the relation $\mathrm{div}_{\vec{p}}(\vec{q} \times \vec{p}\,) = (\mathrm{curl}_{\vec{p}}\,\vec{q}\,) \cdot \vec{p} - \vec{q} \cdot (\mathrm{curl}_{\vec{p}}\,\vec{p}\,) = \vec{0}$ and analogously for the divergence with respect to $\vec{q}$. Therefore, the whole expression vanishes identically, which means that $\dot{\mathfrak{m}}^{(n)}_{\vec{\Phi}} = \dot{\mathfrak{n}}^{(n)}_{\vec{\Phi}} = \ddot{\mathfrak{m}}^{(n)}_{\vec{\Phi}'} = \ddot{\mathfrak{n}}^{(n)}_{\vec{\Phi}'} = 0$ for all $n \in \mathbb{Z}$.

This concludes the proof. □

From this result which allows to compute the integrals in (4.27b), we can obtain the integrals in (4.27a) by means of the following corollary.

Corollary C.2.2 (Angular Integration of Simplified Dotted-Unprimed Terms)

For any $h \in C^1(\mathbb{R}_0^+, \mathbb{R})$ and for vanishing $\vec{q}$ the upper case in (C.32) reduces to

$$
\int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}\,|) \int\limits_{S^2} \mathrm{d}\Omega_\xi\; \vec{\xi} \cdot \vec{\mathbf{Y}}_{lm}(\theta_p, \varphi_p) \mathrm{e}^{-\mathrm{i}\vec{p}\cdot\vec{\xi}} = 4\pi\mathrm{i} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}\,|) \frac{Y_{lm}(\theta_p, \varphi_p)}{|\vec{p}\,|} \dot{\mathfrak{k}}^{(1)}_{\vec{\mathbf{Y}}} j_{0,1}(|\vec{p}\,| r) \tag{C.39}
$$

where $\dot{\mathfrak{k}}^{(1)}_{\vec{\mathbf{Y}}}$ are entries of the operator-valued, dimensionless (3×1)-matrix $\dot{\mathfrak{k}}^{(1)}$ given by

$$
\dot{\mathfrak{k}}^{(1)} = \begin{pmatrix} r\frac{\mathrm{d}}{\mathrm{d}r} & 0 & 0 \end{pmatrix}^{\mathrm{T}} \tag{C.39a}
$$

Proof. Taking the limit $|\vec{q}\,| \to 0$ in the expression $\sum_{n=1}^{5} \dot{\mathfrak{m}}^{(n)} j_{0,n}(k_\pm r)$ we find for the first component

$$
\begin{aligned}
\lim_{|\vec{q}\,|\to 0} \sum_{n=1}^{5} \dot{\mathfrak{m}}^{(n)}_{\vec{Y}} j_{0,n}(k_\pm r) = \\
&= \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} j_{0,1}(|\vec{p}\,|r) + |\vec{p}\,|^2 r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] j_{0,3}(|\vec{p}\,|r) \\
&\overset{(4.26)}{=} \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} j_{0,1}(|\vec{p}\,|r) + r^2 \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \left(r^{-2} j_{0,1}(|\vec{p}\,|r)\right) = r\frac{\mathrm{d}}{\mathrm{d}r} j_{0,1}(|\vec{p}\,|r) =: \dot{\mathfrak{k}}^{(1)}_{\vec{Y}} j_{0,1}(|\vec{p}\,|r)
\end{aligned} \tag{C.40}
$$

For the second component we similarly obtain

$$
\lim_{|\vec{q}\,|\to 0} \sum_{n=1}^{5} \dot{\mathfrak{m}}^{(n)}_{\vec{\Psi}} j_{0,n}(k_\pm r) =
$$

$$= \left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,1}(|\vec{p}|r) - 2|\vec{p}|^2r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 j_{0,3}(|\vec{p}|r)$$
$$+ |\vec{p}|^4r^4\left[2+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,5}(|\vec{p}|r)$$
$$\overset{(4.26)}{=} \left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]j_{0,1}(|\vec{p}|r) - 2r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 \left(r^{-2}j_{0,1}(|\vec{p}|r)\right)$$
$$+ r^4\left[2+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left(r^{-4}j_{0,1}(|\vec{p}|r)\right)$$
$$= \left[\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] - 2r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\frac{1}{2r}\frac{\mathrm{d}}{\mathrm{d}r} - \left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1-\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\right]j_{0,1}(|\vec{p}|r)$$
$$= \left[2\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 - r\frac{\mathrm{d}}{\mathrm{d}r} - \frac{r^3}{2}\frac{\mathrm{d}}{\mathrm{d}r}\left[\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right]\right]j_{0,1}(|\vec{p}|r) = 0 \tag{C.41}$$

which means that $\dot{\mathfrak{k}}^{(1)}_{\vec{\Psi}} = 0$. Together with $\dot{\mathfrak{k}}^{(1)}_{\vec{\Phi}} = 0$ we therefore end up with

$$\dot{\mathfrak{k}}^{(1)} = \begin{pmatrix} r\frac{\mathrm{d}}{\mathrm{d}r} & 0 & 0\end{pmatrix}^{\mathrm{T}} \tag{C.42}$$

which concludes the proof. □

C.3 Evaluation of Double-Dotted Terms

The computation of the position space angular integral (4.27b) in Proposition 4.2.4 (Position Space Angular Integration of Υ_{lm}, $\Upsilon_{lm|l'm'}$, $\mathring{\Upsilon}_{lm|l'm'}$) requires to evaluate integrals of the form

$$\int_{S^2} \mathrm{d}\Omega_\xi \, \left(\vec{\xi}\cdot\vec{\mathbf{Y}}_{lm}(\theta_p,\varphi_p)\right)\left(\vec{\xi}\cdot\vec{\mathbf{Y}}_{l'm'}(\theta_q,\varphi_q)\right)\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} \quad \text{with} \quad \vec{\mathbf{Y}}_{l^{(\prime)}m^{(\prime)}} \in \{\vec{Y}_{l^{(\prime)}m^{(\prime)}}, \vec{\Phi}_{l^{(\prime)}m^{(\prime)}}, \vec{\Psi}_{l^{(\prime)}m^{(\prime)}}\}$$

which correspond to the *double-dotted* terms of $\Upsilon_{lm|l'm'}$. All these integrals can be computed systematically using the following lemma.

Lemma C.3.1 (Angular Integration of Double-Dotted Terms)

For any functions $h, k \in C^1(\mathbb{R}_0^+, \mathbb{R})$ and for $\vec{\mathbf{Y}}_{l^{(\prime)}m^{(\prime)}} \in \{\vec{Y}_{l^{(\prime)}m^{(\prime)}}, \vec{\Phi}_{l^{(\prime)}m^{(\prime)}}, \vec{\Psi}_{l^{(\prime)}m^{(\prime)}}\}$ the relation

$$\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \int_{S^2} \mathrm{d}\Omega_\xi \, \left(\vec{\xi}\cdot\vec{\mathbf{Y}}_{lm}(\theta_p,\varphi_p)\right)\left(\vec{\xi}\cdot\vec{\mathbf{Y}}_{l'm'}(\theta_q,\varphi_q)\right)\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} =$$
$$= 4\pi \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \frac{Y_{lm}(\theta_p,\varphi_p)}{|\vec{p}|}\frac{Y_{l'm'}(\theta_q,\varphi_q)}{|\vec{q}|} \sum_{n=1}^{5} \begin{cases} \ddot{\mathfrak{m}}^{(n)}_{\vec{\mathbf{Y}}\vec{\mathbf{Y}}'} j_{0,n}(k_+r) \\ \ddot{\mathfrak{n}}^{(n)}_{\vec{\mathbf{Y}}\vec{\mathbf{Y}}'} j_{0,n}(k_-r) \end{cases} \tag{C.43}$$

holds, where the sum runs only over odd indices and where $\ddot{\mathfrak{m}}^{(n)}_{\vec{\mathbf{Y}}\vec{\mathbf{Y}}'}$ and $\ddot{\mathfrak{n}}^{(n)}_{\vec{\mathbf{Y}}\vec{\mathbf{Y}}'}$ are entries of operator-valued, dimensionless (3×3)-matrices $\ddot{\mathfrak{m}}^{(n)}$ and $\ddot{\mathfrak{n}}^{(n)}$. The non-vanishing matrices are explicitly given by

$$\begin{Bmatrix} \ddot{\mathfrak{m}}^{(1)} \\ \ddot{\mathfrak{n}}^{(1)} \end{Bmatrix} = \begin{Bmatrix} -1 \\ +1 \end{Bmatrix} \begin{pmatrix} \left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 & l(l+1)\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] & 0 \\ l'(l'+1)\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] & -l(l+1)l'(l'+1) & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{C.43a}$$

$$\begin{Bmatrix} \ddot{\mathfrak{m}}^{(3)} \\ \ddot{\mathfrak{n}}^{(3)} \end{Bmatrix} = \begin{Bmatrix} +1 \\ -1 \end{Bmatrix} \begin{pmatrix} (|\vec{p}|^2+|\vec{q}|^2) & -l'(l'+1)(|\vec{p}|^2-|\vec{q}|^2) & 0 \\ l(l+1)(|\vec{p}|^2-|\vec{q}|^2) & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} r^2 \left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.43b}$$

$$\begin{Bmatrix} \ddot{\mathfrak{m}}^{(5)} \\ \ddot{\mathfrak{n}}^{(5)} \end{Bmatrix} = \begin{Bmatrix} +1 \\ -1 \end{Bmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} (|\vec{p}|^2-|\vec{q}|^2)^2 r^4 \left[2+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.43c}$$

Proof. The guiding principle of this proof is to first rewrite factors of $\vec{\xi}$ as gradients of the exponential factor with respect to $\vec{p}$ and $\vec{q}$, respectively, as we already did in Lemma C.2.1, and subsequently to carry out the position space angular integral using Proposition C.1.1. Afterwards, whenever necessary, we integrate by parts with respect to $\vec{p}$ and $\vec{q}$ in order to achieve that spherical harmonics appear with an even number of gradients acting on them.

(1) $\vec{\mathbf{Y}}_{lm} = \vec{Y}_{lm}$ and $\vec{\mathbf{Y}}_{l'm'} \in \{\vec{Y}_{l'm'}, \vec{\Psi}_{l'm'}, \vec{\Phi}_{l'm'}\}$

We start by fixing $\vec{\mathbf{Y}}_{lm}$ as the radial vector spherical harmonic $\vec{\mathbf{Y}}_{lm} = \vec{Y}_{lm}$ and systematically consider all possible choices for $\vec{\mathbf{Y}}_{l'm'}$.

(a) $\vec{\mathbf{Y}}_{l'm'} = \vec{Y}_{l'm'}$

In the first case we find

$$\int_{S^2} \mathrm{d}\Omega_\xi \, \big(\vec{\xi}\cdot\vec{Y}_{lm}(\theta_p,\varphi_p)\big)\big(\vec{\xi}\cdot\vec{Y}_{l'm'}(\theta_q,\varphi_q)\big)\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} =$$
$$\overset{\text{(C.1)}}{=} \mp 4\pi\big(\vec{Y}_{lm}(\theta_p,\varphi_p)\cdot\mathrm{grad}_{\vec{p}}\big)\big(\vec{Y}_{l'm'}(\theta_q,\varphi_q)\cdot\mathrm{grad}_{\vec{q}}\big) j_{0,1}(k_\pm r)$$

Inserting the definition of $\vec{Y}_{lm}$ and observing that the gradient with respect to $\vec{p}$ does not act on $\vec{Y}_{l'm'}(\theta_q,\varphi_q)$ gives

$$\cdots = \mp 4\pi \frac{Y_{lm}}{|\vec{p}|}\frac{Y_{l'm'}}{|\vec{q}|}\big(\vec{p}\cdot\mathrm{grad}_{\vec{p}}\big)\big(\vec{q}\cdot\mathrm{grad}_{\vec{q}}\big) j_{0,1}(k_\pm r)$$

By inserting the result from Auxiliary Calculation C.1.5 for the two-fold gradient of $j_{0,1}(k_\pm r)$ we find

$$\int_{S^2} \mathrm{d}\Omega_\xi \, \big(\vec{\xi}\cdot\vec{Y}_{lm}(\theta_p,\varphi_p)\big)\big(\vec{\xi}\cdot\vec{Y}_{l'm'}(\theta_q,\varphi_q)\big)\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} =$$
$$\overset{\text{(C.24)}}{=} 4\pi \frac{Y_{lm}}{|\vec{p}|}\frac{Y_{l'm'}}{|\vec{q}|} \sum_{n=1}^{5} \begin{Bmatrix} \ddot{\mathfrak{m}}^{(n)}_{\vec{Y}\vec{Y}'} j_{0,n}(k_+ r) \\ \ddot{\mathfrak{n}}^{(n)}_{\vec{Y}\vec{Y}'} j_{0,n}(k_- r) \end{Bmatrix} \tag{C.44}$$

where $\ddot{\mathfrak{m}}^{(n)}_{\vec{Y}\vec{Y}'}$ and $\ddot{\mathfrak{m}}^{(n)}_{\vec{Y}\vec{Y}'}$ are differential operators with respect to r given by

$$\begin{Bmatrix} \ddot{\mathfrak{m}}^{(1)}_{\vec{Y}\vec{Y}'} \\ \ddot{\mathfrak{n}}^{(1)}_{\vec{Y}\vec{Y}'} \end{Bmatrix} = \begin{Bmatrix} -1 \\ +1 \end{Bmatrix} \left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 \tag{C.44a}$$

$$\begin{Bmatrix} \ddot{\mathfrak{m}}^{(3)}_{\vec{Y}\vec{Y}'} \\ \ddot{\mathfrak{n}}^{(3)}_{\vec{Y}\vec{Y}'} \end{Bmatrix} = \begin{Bmatrix} +1 \\ -1 \end{Bmatrix} (|\vec{p}|^2 + |\vec{q}|^2) r^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] \tag{C.44b}$$

$$\begin{Bmatrix} \ddot{\mathfrak{m}}^{(5)}_{\vec{Y}\vec{Y}'} \\ \ddot{\mathfrak{n}}^{(5)}_{\vec{Y}\vec{Y}'} \end{Bmatrix} = \begin{Bmatrix} +1 \\ -1 \end{Bmatrix} (|\vec{p}|^2 - |\vec{q}|^2)^2 r^4 \left[2 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] \tag{C.44c}$$

(b) $\vec{\mathbf{Y}}_{l'm'} = \vec{\Psi}_{l'm'}$

In the second case, namely for $\vec{\mathbf{Y}}_{l'm'} = \vec{\Psi}_{l'm'}$, we find

$$\begin{aligned} &\int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|) \int_{S^2} \mathrm{d}\Omega_\xi\ \big(\vec{\xi} \cdot \vec{Y}_{lm}(\theta_p, \varphi_p)\big)\big(\vec{\xi} \cdot \vec{\Psi}_{l'm'}(\theta_q, \varphi_q)\big) \mathrm{e}^{-\mathrm{i}(\vec{p} \pm \vec{q}) \cdot \vec{\xi}} = \\ &\overset{\text{(C.1)}}{=} \mp 4\pi \frac{Y_{lm}}{|\vec{p}|} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|)|\vec{q}| \big(\operatorname{grad}_{\vec{q}} Y_{l'm'} \cdot \operatorname{grad}_{\vec{q}}\big)\big(\vec{p} \cdot \operatorname{grad}_{\vec{p}}\big) j_{0,1}(k_\pm r) \end{aligned}$$

where we interchanged the two factors $\big(\vec{\xi} \cdot \vec{Y}_{lm}(\theta_p, \varphi_p)\big)$ and $\big(\vec{\xi} \cdot \vec{\Psi}_{l'm'}(\theta_q, \varphi_q)\big)$ before rewriting the factors $\vec{\xi}$ as derivatives of the exponential. Next, in order to arrange that both gradients with respect to $\vec{q}$ act on the spherical harmonic $Y_{l'm'}$, we integrate by parts with respect to $\vec{q}$ and thus obtain

$$\begin{aligned} \cdots = \mp 4\pi \frac{Y_{lm}}{|\vec{p}|} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ \Big[&\operatorname{div}_{\vec{q}} \Big(\vec{p} \cdot \operatorname{grad}_{\vec{p}} j_{0,1}(k_\pm r) k(|\vec{q}|)|\vec{q}| \operatorname{grad}_{\vec{q}} Y_{l'm'} \Big) \\ &- \vec{p} \cdot \operatorname{grad}_{\vec{p}} j_{0,1}(k_\pm r) \operatorname{div}_{\vec{q}} \Big(k(|\vec{q}|)|\vec{q}| \operatorname{grad}_{\vec{q}} Y_{l'm'} \Big) \Big] \end{aligned}$$

Rewriting the first term using the divergence theorem and computing the divergence in the second term results in

$$\begin{aligned} \cdots = &\mp 4\pi \frac{Y_{lm}}{|\vec{p}|} \lim_{|\vec{q}| \to \infty} \Big[k(|\vec{q}|)|\vec{q}|^2 \int_{S^2} \mathrm{d}\Omega_q\ \vec{p} \cdot \operatorname{grad}_{\vec{p}} j_{0,1}(k_\pm r) k(|\vec{q}|) \vec{q} \cdot \operatorname{grad}_{\vec{q}} Y_{l'm'} \Big] \\ &\pm 4\pi \frac{Y_{lm}}{|\vec{p}|} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ \vec{p} \cdot \operatorname{grad}_{\vec{p}} j_{0,1}(k_\pm r) \Big[k'(|\vec{q}|) \vec{q} \cdot \operatorname{grad}_{\vec{q}} Y_{l'm'} + k(|\vec{q}|) \operatorname{div}_{\vec{q}} \big(|\vec{q}| \operatorname{grad}_{\vec{q}} Y_{l'm'} \big) \Big] \end{aligned}$$

As a consequence of the fact that $\operatorname{grad}_{\vec{q}} Y_{l'm'}$ is tangential to S^2, its scalar product with $\vec{q}$ vanishes. Thus, the boundary term and the first term in the second line both disappear such that we are left with

$$\cdots = \pm 4\pi \frac{Y_{lm}}{|\vec{p}|} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|) \vec{p} \cdot \operatorname{grad}_{\vec{p}} j_{0,1}(k_\pm r) \operatorname{div}_{\vec{q}} \big(|\vec{q}| \operatorname{grad}_{\vec{q}} Y_{l'm'} \big)$$

Carrying out the divergence and using $\operatorname{div}_{\vec{q}} \operatorname{grad}_{\vec{q}} Y_{l'm'} = \Delta_{\vec{q}} Y_{l'm'} = -l'(l'+1) \frac{Y_{l'm'}}{|\vec{q}|^2}$, we arrive at

$$\cdots = \pm 4\pi \frac{Y_{lm}}{|\vec{p}|} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|) \vec{p} \cdot \operatorname{grad}_{\vec{p}} j_{0,1}(k_\pm r) \left[\frac{1}{|\vec{q}|} \vec{q} \cdot \operatorname{grad}_{\vec{q}} Y_{l'm'} - |\vec{q}| l'(l'+1) Y_{l'm'} \right]$$

In this expression, the first term again vanishes for orthogonality reasons. Evaluating $\vec{p} \cdot \operatorname{grad}_{\vec{p}} j_{0,1}(k_\pm r)$ using (C.2b) we ultimately end up with

$$\cdots = 4\pi \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ k(|\vec{q}|) \frac{Y_{lm}}{|\vec{p}|} \frac{Y_{l'm'}}{|\vec{q}|} \sum_{n=} \begin{cases} \ddot{\mathfrak{m}}^{(n)}_{\vec{Y}\vec{\Psi}'} j_{0,n}(k_+ r) \\ \ddot{\mathfrak{n}}^{(n)}_{\vec{Y}\vec{\Psi}'} j_{0,n}(k_- r) \end{cases} \tag{C.45a}$$

where the derivative operators are given by

$$\begin{Bmatrix} \ddot{\mathfrak{m}}^{(1)}_{\vec{Y}\vec{\Psi}'} \\ \ddot{\mathfrak{n}}^{(1)}_{\vec{Y}\vec{\Psi}'} \end{Bmatrix} = \begin{Bmatrix} -1 \\ +1 \end{Bmatrix} l'(l'+1)\left[\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.45b}$$

$$\begin{Bmatrix} \ddot{\mathfrak{m}}^{(3)}_{\vec{Y}\vec{\Psi}'} \\ \ddot{\mathfrak{n}}^{(3)}_{\vec{Y}\vec{\Psi}'} \end{Bmatrix} = \begin{Bmatrix} -1 \\ +1 \end{Bmatrix} l'(l'+1)r^2(|\vec{p}|^2 - |\vec{q}|^2)\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.45c}$$

(c) $\vec{\mathbf{Y}}_{l'm'} = \vec{\Phi}_{l'm'}$

In the third case, namely for $\vec{\mathbf{Y}}_{l'm'} = \vec{\Phi}_{l'm'}$, we find

$$\begin{aligned} &\int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|) \int_{S^2} \mathrm{d}\Omega_\xi\ \big(\vec{\xi}\cdot\vec{Y}_{lm}(\theta_p,\varphi_p)\big)\big(\vec{\xi}\cdot\vec{\Phi}_{l'm'}(\theta_q,\varphi_q)\big)\mathrm{e}^{\mp\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} = \\ &\overset{\text{(C.1)}}{=} \mp 4\pi\frac{Y_{lm}}{|\vec{p}|}\int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|)\Big[\big(\vec{q}\times\mathrm{grad}_{\vec{q}}Y_{l'm'}\big)\cdot\mathrm{grad}_{\vec{q}}\Big]\big(\vec{p}\cdot\mathrm{grad}_{\vec{p}}\big)j_{0,1}(k_\pm r) \end{aligned}$$

where we interchanged the two factors $\big(\vec{\xi}\cdot\vec{Y}_{lm}(\theta_p,\varphi_p)\big)$ and $\big(\vec{\xi}\cdot\vec{\Phi}_{l'm'}(\theta_q,\varphi_q)\big)$ before rewriting the factors $\vec{\xi}$ as derivatives of the exponential. Next, in order to arrange that both gradients with respect to $\vec{q}$ act on the spherical harmonic $Y_{l'm'}$, we integrate by parts with respect to $\vec{q}$ and thus obtain

$$\begin{aligned} \cdots = \mp 4\pi\frac{Y_{lm}}{|\vec{p}|}\int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ \Big[&\mathrm{div}_{\vec{q}}\Big(\vec{p}\cdot\mathrm{grad}_{\vec{p}}\,j_{0,1}(k_\pm r)k(|\vec{q}|)\big(\vec{q}\times\mathrm{grad}_{\vec{q}}Y_{l'm'}\big)\Big) \\ &- \vec{p}\cdot\mathrm{grad}_{\vec{p}}\,j_{0,1}(k_\pm r)\mathrm{div}_{\vec{q}}\Big(k(|\vec{q}|)\big(\vec{q}\times\mathrm{grad}_{\vec{q}}Y_{l'm'}\big)\Big)\Big] \end{aligned}$$

Rewriting the first term using the divergence theorem and computing the divergence in the second term results in

$$\begin{aligned} \cdots = &\mp 4\pi\frac{Y_{lm}}{|\vec{p}|}\lim_{|\vec{q}|\to\infty}\Big[k(|\vec{q}|)|\vec{q}|\int_{S^2}\mathrm{d}\Omega_q\ \vec{p}\cdot\mathrm{grad}_{\vec{p}}\,j_{0,1}(k_\pm r)k(|\vec{q}|)\vec{q}\cdot\big(\vec{q}\times\mathrm{grad}_{\vec{q}}Y_{l'm'}\big)\Big] \\ &\pm 4\pi\frac{Y_{lm}}{|\vec{p}|}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\ \vec{p}\cdot\mathrm{grad}_{\vec{p}}\,j_{0,1}(k_\pm r)\Big[\frac{k'(|\vec{q}|)}{|\vec{q}|}\vec{q}\cdot\big(\vec{q}\times\mathrm{grad}_{\vec{q}}Y_{l'm'}\big) \\ &\qquad + k(|\vec{q}|)\mathrm{div}_{\vec{q}}\big(\vec{q}\times\mathrm{grad}_{\vec{q}}Y_{l'm'}\big)\Big] \end{aligned}$$

By exploiting the cyclicity of the triple product $\vec{q}\cdot\big(\vec{q}\times\mathrm{grad}_{\vec{q}}Y_{l'm'}\big)$ and the properties of the cross product, both the boundary term as well as the first term in the second line disappear such that we are left with

$$\cdots = \pm 4\pi\frac{Y_{lm}}{|\vec{p}|}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\ k(|\vec{q}|)\vec{p}\cdot\mathrm{grad}_{\vec{p}}\,j_{0,1}(k_\pm r)\mathrm{div}_{\vec{q}}\big(\vec{q}\times\mathrm{grad}_{\vec{q}}Y_{l'm'}\big) \tag{C.46}$$

Using the relation $\mathrm{div}_{\vec{q}}\big(\vec{q}\times\mathrm{grad}_{\vec{q}}Y_{l'm'}\big) = \big(\mathrm{grad}_{\vec{q}}Y_{l'm'}\big)\cdot\big(\mathrm{curl}_{\vec{q}}\vec{q}\big) - \vec{q}\cdot\big(\mathrm{curl}_{\vec{q}}\,\mathrm{grad}_{\vec{q}}Y_{l'm'}\big)$ together with the fact that both radial vectors and gradients have vanishing curl, it follows that also the remaining term vanishes identically. We thus have $\ddot{\mathfrak{m}}^{(n)}_{\vec{Y}\vec{\Phi}'} = \ddot{\mathfrak{n}}^{(n)}_{\vec{Y}\vec{\Phi}'} = 0$ for all $n\in\mathbb{Z}$.

(2) $\vec{\mathbf{Y}}_{lm} = \vec{\Psi}_{lm}$ and $\vec{\mathbf{Y}}_{l'm'} \in \{\vec{\Psi}_{l'm'}, \vec{\Phi}_{l'm'}\}$

Having gone through all possible choices for $\vec{\mathbf{Y}}_{l'm'}$ for fixed $\vec{\mathbf{Y}}_{lm} = \vec{Y}_{lm}$, we now set $\vec{\mathbf{Y}}_{lm} = \vec{\Psi}_{lm}$ and consider the two possibilities $\vec{\mathbf{Y}}_{l'm'} = \vec{\Psi}_{l'm'}$ and $\vec{\mathbf{Y}}_{l'm'} = \vec{\Phi}_{l'm'}$ one after the other. Due to the fact that in both cases all involved spherical harmonics carry a derivative, we can no longer suppress one of the momentum integrals.

(a) $\vec{\mathbf{Y}}_{l'm'} = \vec{\Psi}_{l'm'}$

Inserting the definitions of $\vec{\Psi}_{lm}$ and $\vec{\Psi}_{l'm'}$ yields

$$\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|) \int_{S^2} \mathrm{d}\Omega_\xi\ \big(\vec{\xi}\cdot\vec{\Psi}_{lm}(\theta_p,\varphi_p)\big)\big(\vec{\xi}\cdot\vec{\Psi}_{l'm'}(\theta_q,\varphi_q)\big)\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} =$$

$$= \mp 4\pi \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|)|\vec{p}| \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|)|\vec{q}| \big(\operatorname{grad}_{\vec{p}} Y_m \cdot \operatorname{grad}_{\vec{p}}\big)\big(\operatorname{grad}_{\vec{q}} Y_{l'm'} \cdot \operatorname{grad}_{\vec{q}}\big) j_{0,1}(k_\pm r)$$

Integrating by parts with respect to $\vec{p}$ in order to make both gradients with respect to $\vec{p}$ act on Y_{lm} yields

$$\cdots = \mp 4\pi \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|)|\vec{q}| \Big[\operatorname{div}_{\vec{p}}\Big(h(|\vec{p}|)|\vec{p}| \operatorname{grad}_{\vec{p}} Y_{lm}\big(\operatorname{grad}_{\vec{q}} Y_{l'm'} \cdot \operatorname{grad}_{\vec{q}}\big) j_{0,1}(k_\pm r)\Big) - \operatorname{grad}_{\vec{q}} Y_{l'm'} \cdot \operatorname{grad}_{\vec{q}} j_{0,1}(k_\pm r) \operatorname{div}_{\vec{p}}\Big(h(|\vec{p}|)|\vec{p}| \operatorname{grad}_{\vec{p}} Y_{lm}\Big)\Big]$$

Rewriting the first term using the divergence theorem and computing the divergence in the second term turns the expression into the following form

$$\cdots = \mp 4\pi \lim_{|\vec{p}|\to\infty} \Big[h(|\vec{p}|)|\vec{p}|^2 \int_{S^2} \mathrm{d}\Omega_p \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|)|\vec{q}|\vec{p}\cdot \operatorname{grad}_{\vec{p}} Y_{lm}\big(\operatorname{grad}_{\vec{q}} Y_{l'm'} \cdot \operatorname{grad}_{\vec{q}}\big) j_{0,1}(k_\pm r)\Big]$$
$$\pm 4\pi \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|)|\vec{q}| \operatorname{grad}_{\vec{q}} Y_{l'm'} \cdot \operatorname{grad}_{\vec{q}} j_{0,1}(k_\pm r) \Big[\frac{\big(h(|\vec{p}|)|\vec{p}|\big)'}{|\vec{p}|}\vec{p}\cdot \operatorname{grad}_{\vec{p}} Y_{lm} + h(|\vec{p}|)|\vec{p}| \operatorname{div}_{\vec{p}} \operatorname{grad}_{\vec{p}} Y_{lm}\Big]$$

By the same reasoning employed earlier, namely due to the orthogonality of $\vec{p}$ and $\operatorname{grad}_{\vec{p}} Y_{lm}$, the boundary term as well as the first term in the second line vanish. Furthermore, by using $\operatorname{div}_{\vec{p}} \operatorname{grad}_{\vec{p}} Y_{lm} = -l(l+1)\frac{Y_{lm}}{|\vec{p}|^2}$ we arrive at

$$\cdots = \pm 4\pi l(l+1) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|)\frac{Y_{lm}}{|\vec{p}|} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|)|\vec{q}| \operatorname{grad}_{\vec{q}} Y_{l'm'} \cdot \operatorname{grad}_{\vec{q}} j_{0,1}(k_\pm r)$$

It remains to make both remaining gradients with respect to $\vec{q}$ act on $Y_{l'm'}$. To this end, we again integrate by parts, but now with respect to $\vec{q}$ and thus find

$$\cdots = \pm 4\pi l(l+1) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|)\frac{Y_{lm}}{|\vec{p}|} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ \Big[\operatorname{div}_{\vec{q}}\Big(k(|\vec{q}|)|\vec{q}| \operatorname{grad}_{\vec{q}} Y_{l'm'} j_{0,1}(k_\pm r)\Big) - j_{0,1}(k_\pm r)\operatorname{div}_{\vec{q}}\Big(k(|\vec{q}|)|\vec{q}|\operatorname{grad}_{\vec{q}} Y_{l'm'}\Big)\Big]$$

Rewriting the first term using the divergence theorem and carrying out the divergence in the second term, we are obtain

$$\cdots = \pm 4\pi l(l+1) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|)\frac{Y_{lm}}{|\vec{p}|} \lim_{|\vec{q}|\to\infty} \Big[k(|\vec{q}|)|\vec{q}|^2 \int_{S^2} \mathrm{d}\Omega_q\ \vec{q}\cdot \operatorname{grad}_{\vec{q}} Y_{l'm'} j_{0,1}(k_\pm r)\Big]$$
$$\mp 4\pi l(l+1) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|)\frac{Y_{lm}}{|\vec{p}|} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ j_{0,1}(k_\pm r)\Big[\frac{\big(k(|\vec{q}|)|\vec{q}|\big)'}{|\vec{q}|}\vec{q}\cdot \operatorname{grad}_{\vec{q}} Y_{l'm'} + k(|\vec{q}|)|\vec{q}| \operatorname{div}_{\vec{q}} \operatorname{grad}_{\vec{q}} Y_{l'm'}\Big]$$

Once more, the terms containing $\vec{q}\cdot\text{grad}_{\vec{q}}Y_{l'm'}$ vanish due to orthogonality. Using the relation $\text{div}_{\vec{q}}\,\text{grad}_{\vec{q}}Y_{l'm'} = \Delta_{\vec{q}}Y_{l'm'} = -l'(l'+1)\frac{Y_{l'm'}}{|\vec{q}|^2}$ we finally end up with

$$\cdots = 4\pi \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)\frac{Y_{lm}}{|\vec{p}|}\frac{Y_{l'm'}}{|\vec{q}|}\begin{cases}\ddot{\mathfrak{m}}^{(1)}_{\Psi\Psi'}j_{0,1}(k_+r)\\ \ddot{\mathfrak{n}}^{(1)}_{\Psi\Psi'}j_{0,1}(k_-r)\end{cases}$$

where the non-vanishing derivative operators are given by

$$\begin{Bmatrix}\ddot{\mathfrak{m}}^{(1)}_{\Psi\Psi'}\\ \ddot{\mathfrak{m}}^{(1)}_{\Psi\Psi'}\end{Bmatrix} = \begin{Bmatrix}+1\\-1\end{Bmatrix} l(l+1)l'(l'+1) \tag{C.47}$$

(b) $\vec{\mathbf{Y}}_{l'm'} = \vec{\Phi}_{l'm'}$

Inserting the definitions of $\vec{\Psi}_{lm}$ and $\vec{\Phi}_{l'm'}$ yields

$$\int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \int\limits_{S^2} \mathrm{d}\Omega_\xi\; \big(\vec{\xi}\cdot\vec{\Psi}_{lm}(\theta_p,\varphi_p)\big)\big(\vec{\xi}\cdot\vec{\Phi}_{l'm'}(\theta_q,\varphi_q)\big)\mathrm{e}^{\mp\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} =$$
$$= \mp 4\pi \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)|\vec{q}|\big(\,\text{grad}_{\vec{p}}Y_m\cdot\text{grad}_{\vec{p}}\big)\Big(\big(\vec{q}\times\text{grad}_{\vec{q}}Y_{l'm'}\big)\cdot\text{grad}_{\vec{q}}\Big)j_{0,1}(k_\pm r)$$

Integrating by parts with respect to $\vec{p}$ in order to make both gradients with respect to $\vec{p}$ act on Y_{lm} yields

$$\cdots = \mp 4\pi \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)\Big[\text{div}_{\vec{p}}\Big(h(|\vec{p}|)|\vec{p}|\,\text{grad}_{\vec{p}}Y_{lm}\Big(\big(\vec{q}\times\text{grad}_{\vec{q}}Y_{l'm'}\big)\cdot\text{grad}_{\vec{q}}\Big)j_{0,1}(k_\pm r)\Big)$$
$$-\big(\vec{q}\times\text{grad}_{\vec{q}}Y_{l'm'}\big)\cdot\text{grad}_{\vec{q}}j_{0,1}(k_\pm r)\text{div}_{\vec{p}}\Big(h(|\vec{p}|)|\vec{p}|\,\text{grad}_{\vec{p}}Y_{lm}\Big)\Big]$$

Rewriting the first term using the divergence theorem and computing the divergence in the second term turns the expression into the following form

$$\cdots = \mp 4\pi \lim_{|\vec{p}|\to\infty}\Bigg[h(|\vec{p}|)|\vec{p}|^2\int\limits_{S^2}\mathrm{d}\Omega_p \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)|\vec{q}|\big(\vec{p}\cdot\text{grad}_{\vec{p}}Y_{lm}\big)$$
$$\Big(\big(\vec{q}\times\text{grad}_{\vec{q}}Y_{l'm'}\big)\cdot\text{grad}_{\vec{q}}\Big)j_{0,1}(k_\pm r)\Bigg]$$
$$\pm 4\pi \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)\big(\vec{q}\times\text{grad}_{\vec{q}}Y_{l'm'}\big)\cdot$$
$$\cdot\,\text{grad}_{\vec{q}}j_{0,1}(k_\pm r)\left[\frac{\big(h(|\vec{p}|)|\vec{p}|\big)'}{|\vec{p}|}\vec{p}\cdot\text{grad}_{\vec{p}}Y_{lm} + h(|\vec{p}|)|\vec{p}|\text{div}_{\vec{p}}\,\text{grad}_{\vec{p}}Y_{lm}\right]$$

Once more, due to the orthogonality of $\vec{p}$ and $\text{grad}_{\vec{p}}Y_{lm}$, the boundary term as well as the first term in the second line vanish. Using $\text{div}_{\vec{p}}\,\text{grad}_{\vec{p}}Y_{lm} = -l(l+1)\frac{Y_{lm}}{|\vec{p}|^2}$ the remaining part reads

$$\cdots = \mp 4\pi l(l+1)\int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)\frac{Y_{lm}}{|\vec{p}|}\int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)\big(\vec{q}\times\text{grad}_{\vec{q}}Y_{l'm'}\big)\cdot\text{grad}_{\vec{q}}j_{0,1}(k_\pm r)$$

In order get rid of the gradient with respect to $\vec{q}$ acting on the spherical harmonic $Y_{l'm'}$ we first exploit the cyclicity of the triple product and subsequently integrate by parts with respect to $\vec{q}$. We find

$$\cdots = \mp 4\pi l(l+1)\int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)\frac{Y_{lm}}{|\vec{p}|}\int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\;\Big[\text{div}_{\vec{q}}\Big(Y_{l'm'}k(|\vec{q}|)\big(\,\text{grad}_{\vec{q}}j_{0,1}(k_\pm r)\times\vec{q}\big)\Big)$$
$$-Y_{l'm'}\text{div}_{\vec{q}}\Big(k(|\vec{q}|)\text{grad}_{\vec{q}}j_{0,1}(k_\pm r)\times\vec{q}\Big)\Big]$$

Rewriting the first term using the divergence theorem and carrying out the divergence in the second term, we arrive at

$$\cdots = \mp 4\pi l(l+1) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \frac{Y_{lm}}{|\vec{p}|} \lim_{|\vec{q}|\to\infty} \left[k(|\vec{q}|)|\vec{q}|^2 \int_{S^2} \mathrm{d}\Omega_q \; \frac{Y_{l'm'}}{|\vec{q}|} \vec{q} \cdot \big(\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) \times \vec{q} \big) \right]$$
$$\pm 4\pi l(l+1) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \frac{Y_{lm}}{|\vec{p}|} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{l'm'} \left[\frac{\big(k(|\vec{q}|)|\vec{q}|\big)'}{|\vec{q}|} \vec{q} \cdot \big(\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) \times \vec{q} \big) + k(|\vec{q}|)|\vec{q}| \mathrm{div}_{\vec{q}} \big(\mathrm{grad}_{\vec{q}} j_{0,1}(k_\pm r) \times \vec{q} \big) \right]$$

According to the properties of the triple product and the cross product, terms containing the factor $\vec{q} \cdot \big(\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) \times \vec{q} \big)$ vanish such that only the last term remains

$$\cdots = \pm 4\pi l(l+1) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \frac{Y_{lm}}{|\vec{p}|} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \frac{Y_{l'm'}}{|\vec{q}|} |\vec{q}|^2 \mathrm{div}_{\vec{q}} \big(\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) \times \vec{q} \big)$$

To simplify this expression, we use (C.2a) and find

$$\cdots = \mp 4\pi l(l+1) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \frac{Y_{lm}}{|\vec{p}|} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \frac{Y_{l'm'}}{|\vec{q}|} |\vec{q}|^2 \, \mathrm{div}_{\vec{q}} \left(\pm 2(\vec{p} \times \vec{q}) r^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] j_{0,3}(k_\pm r) \right)$$

Carrying out the divergence, we obtain

$$\cdots = -8\pi r^2 l(l+1) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \frac{Y_{lm}}{|\vec{p}|} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \frac{Y_{l'm'}}{|\vec{q}|} |\vec{q}|^2 \left[1 + \frac{r}{2} \frac{\mathrm{d}}{\mathrm{d}r} \right] \times \times \left[\mathrm{div}_{\vec{q}} (\vec{p} \times \vec{q}) j_{0,3}(k_\pm r) + (\vec{p} \times \vec{q}) \cdot \mathrm{grad}_{\vec{q}}\, j_{0,3}(k_\pm r) \right] \tag{C.48}$$

The first term in this expression vanishes due to the relation $\mathrm{div}_{\vec{q}}(\vec{p} \times \vec{q}) = (\mathrm{curl}_{\vec{q}} \vec{p}) \cdot \vec{q} - \vec{p} \cdot (\mathrm{curl}_{\vec{q}} \vec{q}) \cdot \vec{q} = \vec{0}$ while the second term vanishes as a consequence of the fact that $\mathrm{grad}_{\vec{q}}\, j_{0,n}(k_\pm r) \propto (\vec{p} \pm \vec{q})$ together with the properties of the triple product. All in all the whole expression vanishes which means that $\ddot{\mathfrak{m}}^{(n)}_{\vec{\Psi}\vec{\Phi}'} = 0$ and $\ddot{\mathfrak{n}}^{(n)}_{\vec{\Psi}\vec{\Phi}'} = 0$ for all $n \in \mathbb{Z}$.

(3) $\vec{\mathbf{Y}}_{lm} = \vec{\Phi}_{lm}$ and $\vec{\mathbf{Y}}_{l'm'} = \vec{\Phi}_{l'm'}$

Finally, we fix $\vec{\mathbf{Y}}_{lm} = \vec{\Phi}_{lm}$ and consider the only remaining case $\vec{\mathbf{Y}}_{l'm'} = \vec{\Phi}_{l'm'}$. Inserting the definitions, we obtain

$$\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \int_{S^2} \mathrm{d}\Omega_\xi \; \big(\vec{\xi} \cdot \vec{\Phi}_{lm}(\theta_p, \varphi_p)\big)\big(\vec{\xi} \cdot \vec{\Phi}_{l'm'}(\theta_q, \varphi_q)\big) \mathrm{e}^{-\mathrm{i}(\vec{p} \pm \vec{q}) \cdot \vec{\xi}} =$$
$$= \mp 4\pi \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \Big(\big(\vec{p} \times \mathrm{grad}_{\vec{p}} Y_m\big) \cdot \mathrm{grad}_{\vec{p}} \Big) \Big(\big(\vec{q} \times \mathrm{grad}_{\vec{q}} Y_{l'm'}\big) \cdot \mathrm{grad}_{\vec{q}} \Big) j_{0,1}(k_\pm r)$$

Integrating by parts with respect to $\vec{p}$ yields

$$\cdots = \mp 4\pi \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \Big[\mathrm{div}_{\vec{p}} \Big(h(|\vec{p}|) \vec{p} \times \mathrm{grad}_{\vec{p}} Y_{lm} \Big(\big(\vec{q} \times \mathrm{grad}_{\vec{q}} Y_{l'm'}\big) \cdot \mathrm{grad}_{\vec{q}} \Big) j_{0,1}(k_\pm r) \Big) - \big(\vec{q} \times \mathrm{grad}_{\vec{q}} Y_{l'm'}\big) \cdot \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) \mathrm{div}_{\vec{p}} \Big(h(|\vec{p}|) \vec{p} \times \mathrm{grad}_{\vec{p}} Y_{lm} \Big) \Big]$$

Rewriting the first term using the divergence theorem and computing the divergence in the second term turns the expression into the following form

$$\begin{aligned}\cdots = \mp 4\pi \lim_{|\vec{p}|\to\infty} \Bigg[h(|\vec{p}|)|\vec{p}|^2 \int\limits_{S^2} \mathrm{d}\Omega_p \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)|\vec{q}|\vec{p}\cdot\big(\vec{p}\times\mathrm{grad}_{\vec{p}}Y_{lm}\big)\times \\ \Big(\big(\vec{q}\times\mathrm{grad}_{\vec{q}}Y_{l'm'}\big)\cdot\mathrm{grad}_{\vec{q}}\Big)j_{0,1}(k_\pm r)\Bigg] \\ \pm 4\pi \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)\big(\vec{q}\times\mathrm{grad}_{\vec{q}}Y_{l'm'}\big)\cdot\mathrm{grad}_{\vec{q}}\,j_{0,1}(k_\pm r)\times \\ \times\left[\frac{h'(|\vec{p}|)}{|\vec{p}|}\vec{p}\cdot\big(\vec{p}\times\mathrm{grad}_{\vec{p}}Y_{lm}\big) + h(|\vec{p}|)\mathrm{div}_{\vec{p}}\big(\vec{p}\times\mathrm{grad}_{\vec{p}}Y_{lm}\big)\right]\end{aligned} \tag{C.49}$$

Due to the cyclicity of the triple product and the properties of the cross product, terms containing $\vec{p}\cdot\big(\vec{p}\times\mathrm{grad}_{\vec{p}}Y_{lm}\big)$ vanish. The remaining term also vanishes as can be seen by using the relation $\mathrm{div}_{\vec{p}}\big(\vec{p}\times\mathrm{grad}_{\vec{p}}Y_{lm}\big) = \big(\mathrm{curl}_{\vec{p}}\vec{p}\big)\cdot\mathrm{grad}_{\vec{q}}Y_{lm} - \vec{p}\cdot\mathrm{curl}_{\vec{p}}\,\mathrm{grad}_{\vec{p}}Y_{lm}$ and recalling that both the curl of a radial vector as well as the curl of a gradient vanish identically. We thus have $\ddot{\mathfrak{m}}^{(n)}_{\vec{\Phi}\vec{\Phi}'} = 0$ and $\ddot{\mathfrak{n}}^{(n)}_{\vec{\Phi}\vec{\Phi}'} = 0$ for all $n\in\mathbb{Z}$.

Up to this point the we have only determined the entries of the operator-valued matrices $\ddot{\mathfrak{m}}^{(n)}$ and $\ddot{\mathfrak{n}}^{(n)}$ lying on or above the diagonal. By simultaneously interchanging the functions $h\leftrightarrow k$, the variables $\vec{p}\leftrightarrow\vec{q}$ and the parameters $(l,m)\leftrightarrow(l'm')$ the expression

$$\int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \int\limits_{S^2} \mathrm{d}\Omega_\xi\; \big(\vec{\xi}\cdot\vec{\mathbf{Y}}_{lm}(\theta_p,\varphi_p)\big)\big(\vec{\xi}\cdot\vec{\mathbf{Y}}_{l'm'}(\theta_q,\varphi_q)\big)\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} \tag{C.50}$$

remains unchanged except for an additional factor (± 1) appearing in the exponential. However, due to Proposition C.1.1 this factor disappears upon carrying out the position space angular integral. As a consequence, the entries of the matrices $\ddot{\mathfrak{m}}^{(n)}$ and $\ddot{\mathfrak{n}}^{(n)}$ below the diagonal can be found by interchanging $\vec{p}\leftrightarrow\vec{q}$ and $(l,m)\leftrightarrow(l'm')$ in the corresponding entries above the diagonal.

This concludes the proof. □

C.4 Evaluation of Asterisked Terms

The computation of the position space angular integral (4.27c) in Proposition 4.2.4 (Position Space Angular Integration of Υ_{lm}, $\Upsilon_{lm|l'm'}$, $\overset{*}{\Upsilon}_{lm|l'm'}$) requires to evaluate integrals of the form

$$\int\limits_{S^2} \mathrm{d}\Omega_\xi\; \vec{\mathbf{Y}}_{lm}(\theta_p,\varphi_p)\cdot\vec{\mathbf{Y}}_{l'm'}(\theta_q,\varphi_q)\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} \quad \text{with} \quad \vec{\mathbf{Y}}_{l^{(\prime)}m^{(\prime)}} \in \{\vec{Y}_{l^{(\prime)}m^{(\prime)}}, \vec{\Phi}_{l^{(\prime)}m^{(\prime)}}, \vec{\Psi}_{l^{(\prime)}m^{(\prime)}}\}$$

which correspond to the matrix $\overset{*}{\Upsilon}_{lm|l'm'}$. All these integrals can be computed systematically using the following lemma.

Lemma C.4.1 (Angular Integration of Asterisked Terms)

For any functions $h,k\in C^1(\mathbb{R}^+_0,\mathbb{R})$ and for $\vec{\mathbf{Y}}_{l^{(\prime)}m^{(\prime)}} \in \{\vec{Y}_{l^{(\prime)}m^{(\prime)}}, \vec{\Phi}_{l^{(\prime)}m^{(\prime)}}, \vec{\Psi}_{l^{(\prime)}m^{(\prime)}}\}$ the relation

$$\int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \int\limits_{S^2} \mathrm{d}\Omega_\xi\; \vec{\mathbf{Y}}_{lm}(\theta_p,\varphi_p)\cdot\vec{\mathbf{Y}}_{l'm'}(\theta_q,\varphi_q)\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} =$$

$$= 4\pi \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|) \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|) Y_{lm} Y_{l'm'} \sum_{\substack{n=-1 \\ n \text{ odd}}}^{5} \begin{cases} \overset{*}{\mathfrak{m}}^{(n)}_{\vec{\mathbf{Y}}\vec{\mathbf{Y}}'} j_{0,n}(k_+ r) \\ \overset{*}{\mathfrak{n}}^{(n)}_{\vec{\mathbf{Y}}\vec{\mathbf{Y}}'} j_{0,n}(k_- r) \end{cases} \tag{C.51}$$

holds, where $\overset{*}{\mathfrak{m}}^{(n)}_{\vec{\mathbf{Y}}\vec{\mathbf{Y}}'}$ and $\overset{*}{\mathfrak{n}}^{(n)}_{\vec{\mathbf{Y}}\vec{\mathbf{Y}}'}$ are entries of operator-valued, dimensionless (3×3)-matrices $\overset{*}{\mathfrak{m}}^{(n)}$ and $\overset{*}{\mathfrak{n}}^{(n)}$, respectively, which are explicitly given by

$$\begin{Bmatrix} \overset{*}{\mathfrak{m}}^{(-1)} \\ \overset{*}{\mathfrak{n}}^{(-1)} \end{Bmatrix} = \begin{Bmatrix} +1 \\ -1 \end{Bmatrix} \frac{1}{2|\vec{p}||\vec{q}|r^2} \begin{pmatrix} 1 & \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] & 0 \\ \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] & \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{C.51a}$$

$$\begin{Bmatrix} \overset{*}{\mathfrak{m}}^{(1)} \\ \overset{*}{\mathfrak{n}}^{(1)} \end{Bmatrix} = \begin{Bmatrix} -1 \\ +1 \end{Bmatrix} \frac{|\vec{p}|^2 + |\vec{q}|^2}{|\vec{p}||\vec{q}|} \begin{pmatrix} \frac{1}{2} & \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] & 0 \\ \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] & \left[2 + \frac{3r}{4}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{C.51b}$$

$$\begin{Bmatrix} \overset{*}{\mathfrak{m}}^{(3)} \\ \overset{*}{\mathfrak{n}}^{(3)} \end{Bmatrix} = \begin{Bmatrix} +1 \\ -1 \end{Bmatrix} \frac{(|\vec{p}|^2 - |\vec{q}|^2)^2}{|\vec{p}||\vec{q}|} r^2 \begin{pmatrix} 0 & 1 & 0 \\ 1 & 1 + \frac{2(|\vec{p}|^4 + |\vec{q}|^4) + (|\vec{p}|^2 + |\vec{q}|^2)^2}{2(|\vec{p}|^2 - |\vec{q}|^2)^2}\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] & 0 \\ 0 & 0 & 0 \end{pmatrix} \left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.51c}$$

$$\begin{Bmatrix} \overset{*}{\mathfrak{m}}^{(5)} \\ \overset{*}{\mathfrak{n}}^{(5)} \end{Bmatrix} = \begin{Bmatrix} -1 \\ +1 \end{Bmatrix} \frac{(|\vec{p}|^2 + |\vec{q}|^2)(|\vec{p}|^2 - |\vec{q}|^2)^2}{2|\vec{p}||\vec{q}|} r^4 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \left[2 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.51d}$$

Proof. The guiding principle in this proof is similar to the one in Lemma C.2.1: First, we carry out the position space angular integral using Proposition C.1.1 before we start to remove all derivatives from the spherical harmonics via repeated integration by parts with respect to $\vec{p}$ and $\vec{q}$. As a consequence of this procedure, the derivatives reappear as $h'(|\vec{p}|)$ and $k'(|\vec{q}|)$ which in turn have to be removed via integrating by parts with respect to $|\vec{p}|$ and $|\vec{q}|$.

We start by computing the position space angular integral. Due to the fact that only the exponential factor carries a dependence on the variables $(\theta_\xi, \varphi_\xi)$, the corresponding integration can be carried out trivially such that we obtain

$$\int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|) \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|) \int\limits_{S^2} \mathrm{d}\Omega_\xi\ \vec{\mathbf{Y}}_{lm}(\theta_p, \varphi_p) \cdot \vec{\mathbf{Y}}_{l'm'}(\theta_q, \varphi_q) \mathrm{e}^{-\mathrm{i}(\vec{p} \pm \vec{q}) \cdot \vec{\xi}} =$$

$$= 4\pi \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\ h(|\vec{p}|) \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\ k(|\vec{q}|) \vec{\mathbf{Y}}_{lm}(\theta_p, \varphi_p) \cdot \vec{\mathbf{Y}}_{l'm'}(\theta_q, \varphi_q) j_{0,1}(k_\pm r) \tag{C.52}$$

In what follows, we systematically consider all possible combinations of scalar products of $\vec{\mathbf{Y}}_{lm} \in \{\vec{Y}_{lm}, \vec{\Psi}_{lm}, \vec{\Phi}_{lm}\}$ and $\vec{\mathbf{Y}}_{l'm'} \in \{\vec{Y}_{l'm'}, \vec{\Psi}_{l'm'}, \vec{\Phi}_{l'm'}\}$. The order of calculation is as follows:

(1) $\vec{\mathbf{Y}}_{lm} = \vec{Y}_{lm}$ **and** $\vec{\mathbf{Y}}_{l'm'} \in \{\vec{Y}_{l'm'}, \vec{\Psi}_{l'm'}, \vec{\Phi}_{l'm'}\}$

(2) $\vec{\mathbf{Y}}_{lm} = \vec{\Psi}_{lm}$ **and** $\vec{\mathbf{Y}}_{l'm'} \in \{\vec{\Psi}_{l'm'}, \vec{\Phi}_{l'm'}\}$

(3) $\vec{\mathbf{Y}}_{lm} = \vec{\Phi}_{lm}$ **and** $\vec{\mathbf{Y}}_{l'm'} = \vec{\Phi}_{l'm'}$

At the end of the proof a symmetry argument will extend the validity of the following calculations to the missing combinations.

(1) $\vec{\mathbf{Y}}_{lm} = \vec{Y}_{lm}$ and $\vec{\mathbf{Y}}_{l'm'} \in \{\vec{Y}_{l'm'}, \vec{\Psi}_{l'm'}, \vec{\Phi}_{l'm'}\}$

We start by fixing $\vec{\mathbf{Y}}_{lm}$ as the radial vector spherical harmonic $\vec{\mathbf{Y}}_{lm} = \vec{Y}_{lm}$ and systematically consider all possible choices for $\vec{\mathbf{Y}}_{l'm'}$.

(a) $\vec{\mathbf{Y}}_{l'm'} = \vec{Y}_{l'm'}$

In the first case, namely for $\vec{\mathbf{Y}}_{l'm'} = \vec{Y}_{l'm'}$, we do not need any momentum space integrals as there are no derivatives of the spherical harmonics involved. Thus, inserting the definitions of $\vec{Y}_{lm}$ and $\vec{Y}_{l'm'}$ into (C.52) and making use of the relation $k_\pm^2 = |\vec{p}|^2 + |\vec{q}|^2 \pm 2\vec{p}\cdot\vec{q}$, we immediately obtain

$$\begin{aligned}\int\limits_{S^2} \mathrm{d}\Omega_\xi\ \vec{Y}_{lm}\cdot\vec{Y}_{l'm'} j_{0,1}(k_\pm r) &= Y_{lm}Y_{l'm'}\frac{\vec{p}\cdot\vec{q}}{|\vec{p}||\vec{q}|}\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} \\ &= Y_{lm}Y_{l'm'}\left(\pm\frac{k_\pm^2 - |\vec{p}|^2 - |\vec{q}|^2}{2|\vec{p}||\vec{q}|}\right) j_{0,1}(k_\pm r) \\ &= Y_{lm}Y_{l'm'}\sum_{\substack{n=-1\\ n\ \text{odd}}}^{1}\begin{cases}\overset{*}{\mathfrak{m}}^{(n)}_{\vec{Y}\vec{Y}'} j_{0,n}(k_+ r)\\ \overset{*}{\mathfrak{n}}^{(n)}_{\vec{Y}\vec{Y}'} j_{0,n}(k_- r)\end{cases}\end{aligned} \tag{C.53}$$

where $\overset{*}{\mathfrak{m}}^{(n)}_{\vec{Y}\vec{Y}'}$ and $\overset{*}{\mathfrak{n}}^{(n)}_{\vec{Y}\vec{Y}'}$ are differential operators with respect to r given by

$$\begin{Bmatrix}\overset{*}{\mathfrak{m}}^{(-1)}_{\vec{Y}\vec{Y}'}\\ \overset{*}{\mathfrak{n}}^{(-1)}_{\vec{Y}\vec{Y}'}\end{Bmatrix} = \begin{Bmatrix}+1\\ -1\end{Bmatrix}\frac{1}{2|\vec{p}||\vec{q}|r^2} \tag{C.53a}$$

$$\begin{Bmatrix}\overset{*}{\mathfrak{m}}^{(1)}_{\vec{Y}\vec{Y}'}\\ \overset{*}{\mathfrak{n}}^{(1)}_{\vec{Y}\vec{Y}'}\end{Bmatrix} = \begin{Bmatrix}-1\\ +1\end{Bmatrix}\frac{|\vec{p}|^2 + |\vec{q}|^2}{2|\vec{p}||\vec{q}|} \tag{C.53b}$$

(b) $\vec{\mathbf{Y}}_{l'm'} = \vec{\Psi}_{l'm'}$

In the second case, namely $\vec{\mathbf{Y}}_{l'm'} = \vec{\Psi}_{l'm'}$, we have to perform one integration by parts with respect to $\vec{q}$ which implies that the $\vec{p}$-integral can be suppressed. Inserting the definitions of $\vec{Y}_{lm}$ and $\vec{\Psi}_{l'm'}$ yields

$$\begin{aligned}&\int\limits_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\ k(|\vec{q}|)\int\limits_{S^2}\mathrm{d}\Omega_\xi\ \vec{Y}_{lm}\cdot\vec{\Psi}_{l'm'}\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} = \\ &\quad = \frac{Y_{lm}}{|\vec{p}|}\int\limits_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\ k(|\vec{q}|)|\vec{q}|\big(\vec{p}\cdot\mathrm{grad}_{\vec{q}}Y_{l'm'}\big) j_{0,1}(k_\pm r)\end{aligned}$$

Integrating by parts with respect to $\vec{q}$ yields

$$\cdots = \frac{Y_{lm}}{|\vec{p}|}\int\limits_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\ \Big[\mathrm{div}_{\vec{q}}\Big(k(|\vec{q}|)|\vec{q}|Y_{l'm'}j_{0,1}(k_\pm r)\vec{p}\Big) - Y_{l'm'}\mathrm{div}_{\vec{q}}\Big(k(|\vec{q}|)|\vec{q}|j_{0,1}(k_\pm r)\vec{p}\Big)\Big]$$

Rewriting the first term using the divergence theorem and converting the divergence in the second term into a gradient by pulling $\vec{p}$ outside, we arrive at

$$\begin{aligned}\cdots &= \frac{Y_{lm}}{|\vec{p}|}\lim_{|\vec{q}|\to\infty}\Big[k(|\vec{q}|)|\vec{q}|^2\int\limits_{S^2}\mathrm{d}\Omega_q\ Y_{l'm'}j_{0,1}(k_\pm r)(\vec{p}\cdot\vec{q})\Big] \\ &\quad - \frac{Y_{lm}}{|\vec{p}|}\int\limits_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\ Y_{l'm'}\Big[(\vec{p}\cdot\vec{q})\frac{\big(k(|\vec{q}|)|\vec{q}|\big)'}{|\vec{q}|}j_{0,1}(k_\pm r) + k(|\vec{q}|)|\vec{q}|\vec{p}\cdot\mathrm{grad}_{\vec{q}}j_{0,1}(k_\pm r)\Big]\end{aligned}$$

In order to get rid of the derivative of $k(|\vec{q}|)$ in the second line, we have to integrate by parts with respect to $|\vec{q}|$ which turns the expression into

$$\begin{aligned}\dots = &\frac{Y_{lm}}{|\vec{p}|}\lim_{|\vec{q}|\to\infty}\left[k(|\vec{q}|)|\vec{q}|^2\int_{S^2}\mathrm{d}\Omega_q\ Y_{l'm'}j_{0,1}(k_\pm r)(\vec{p}\cdot\vec{q})\right]\\ &-\frac{Y_{lm}}{|\vec{p}|}\lim_{|\vec{q}|\to\infty}\left[k(|\vec{q}|)|\vec{q}|^2\int_{S^2}\mathrm{d}\Omega_q\ Y_{l'm'}(\vec{p}\cdot\vec{q})j_{0,1}(k_\pm r)\right]\\ &+\frac{Y_{lm}}{|\vec{p}|}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\ k(|\vec{q}|)Y_{l'm'}\left[\frac{1}{|\vec{q}|}\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\Big[(\vec{p}\cdot\vec{q})|\vec{q}|j_{0,1}(k_\pm r)\Big]-|\vec{q}|\vec{p}\cdot\mathrm{grad}_{\vec{q}}\,j_{0,1}(k_\pm r)\right]\end{aligned}$$

In evaluating the $|\vec{q}|$-integral at its boundaries we exploited the fact that the integrand vanishes at the lower boundary $|\vec{q}|=0$ as $k\in C^1(\mathbb{R}_0^+,\mathbb{R})$. In the resulting expression, the first and second term cancel each other while for the third term we find by using Auxiliary Calculation C.1.6

$$\dots \overset{\text{(C.25)}}{=} \int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\ k(|\vec{q}|)Y_{lm}Y_{l'm'}\sum_{n=-1}^{3}\begin{cases}\overset{*}{\mathfrak{m}}^{(n)}_{\vec{Y}\vec{\Psi}'}j_{0,n}(k_+r)\\ \overset{*}{\mathfrak{n}}^{(n)}_{\vec{Y}\vec{\Psi}'}j_{0,n}(k_-r)\end{cases} \tag{C.54}$$

where

$$\begin{Bmatrix}\overset{*}{\mathfrak{m}}^{(-1)}_{\vec{Y}\vec{\Psi}'}\\ \overset{*}{\mathfrak{n}}^{(-1)}_{\vec{Y}\vec{\Psi}'}\end{Bmatrix} = \begin{Bmatrix}+1\\-1\end{Bmatrix}\frac{1}{2|\vec{p}||\vec{q}|r^2}\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.54a}$$

$$\begin{Bmatrix}\overset{*}{\mathfrak{m}}^{(1)}_{\vec{Y}\vec{\Psi}'}\\ \overset{*}{\mathfrak{n}}^{(1)}_{\vec{Y}\vec{\Psi}'}\end{Bmatrix} = \begin{Bmatrix}-1\\+1\end{Bmatrix}\frac{|\vec{p}|^2+|\vec{q}|^2}{|\vec{p}||\vec{q}|}\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.54b}$$

$$\begin{Bmatrix}\overset{*}{\mathfrak{m}}^{(3)}_{\vec{Y}\vec{\Psi}'}\\ \overset{*}{\mathfrak{n}}^{(3)}_{\vec{Y}\vec{\Psi}'}\end{Bmatrix} = \begin{Bmatrix}+1\\-1\end{Bmatrix}\frac{(|\vec{p}|^2-|\vec{q}|^2)^2}{|\vec{p}||\vec{q}|}r^2\left[1+\frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.54c}$$

(c) $\vec{\mathbf{Y}}_{l'm'} = \vec{\Phi}_{l'm'}$

Just as above, in the third case, namely for $\vec{\mathbf{Y}}_{l'm'} = \vec{\Phi}_{l'm'}$, we have to perform one integration by parts with respect to $\vec{q}$ which implies that again the $\vec{p}$-integral can be suppressed. Inserting the definitions of $\vec{Y}_{lm}$ and $\vec{\Phi}_{l'm'}$ yields

$$\begin{aligned}&\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\ k(|\vec{q}|)\int_{S^2}\mathrm{d}\Omega_\xi\ \vec{Y}_{lm}\cdot\vec{\Phi}_{l'm'}\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} =\\ &\quad=\frac{Y_{lm}}{|\vec{p}|}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\ k(|\vec{q}|)\vec{p}\cdot\big(\vec{q}\times\mathrm{grad}_{\vec{q}}Y_{l'm'}\big)j_{0,1}(k_\pm r)\\ &\quad=\frac{Y_{lm}}{|\vec{p}|}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\ k(|\vec{q}|)\,\mathrm{grad}_{\vec{q}}Y_{l'm'}\cdot(\vec{p}\times\vec{q})j_{0,1}(k_\pm r)\end{aligned}$$

where in the last step we exploited the cyclicity of the triple product. Integrating by parts with respect to $\vec{q}$ yields

$$\dots = \frac{Y_{lm}}{|\vec{p}|}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\ \left[\mathrm{div}_{\vec{q}}\Big(k(|\vec{q}|)(\vec{p}\times\vec{q})Y_{l'm'}j_{0,1}(k_\pm r)\Big)-Y_{l'm'}\mathrm{div}_{\vec{q}}\Big(k(|\vec{q}|)(\vec{p}\times\vec{q})j_{0,1}(k_\pm r)\Big)\right]$$

Rewriting the first term using the divergence theorem and computing the divergence in the second term we are left with

$$\cdots = \frac{Y_{lm}}{|\vec{p}|} \lim_{|\vec{q}|\to\infty} \left[k(|\vec{q}|)|\vec{q}| \int_{S^2} \mathrm{d}\Omega_q \; Y_{l'm'} j_{0,1}(k_\pm r)(\vec{p}\times\vec{q})\cdot\vec{q} \right]$$
$$- \frac{Y_{lm}}{|\vec{p}|} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q} \; Y_{l'm'} \left[\frac{k'(|\vec{q}|)}{|\vec{q}|} \vec{q}\cdot(\vec{p}\times\vec{q}) j_{0,1}(k_\pm r) + k(|\vec{q}|)\mathrm{div}_{\vec{q}}(\vec{p}\times\vec{q}) j_{0,1}(k_\pm r) + k(|\vec{q}|)(\vec{p}\times\vec{q})\cdot \mathrm{grad}_{\vec{q}} j_{0,1}(k_\pm r) \right] \quad \text{(C.55)}$$

In this expression, all terms containing the factor $(\vec{p}\times\vec{q})\cdot\vec{q}$ vanish as a consequence of the properties of the triple product. Recalling that $\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) \propto (\vec{p}\pm\vec{q})$, also the term containing the gradient vanishes by the same reasoning. Finally, the divergence term also vanishes due to the relation $\mathrm{div}_{\vec{q}}(\vec{p}\times\vec{q}) = (\mathrm{curl}_{\vec{q}}\vec{p})\cdot\vec{q} + \vec{p}\cdot(\mathrm{curl}_{\vec{q}}\vec{q}) = \vec{0}$ because $\vec{q}\cdot(\vec{p}\times\vec{q}) = \vec{0}$ and $\vec{q}\cdot(\vec{p}\times\vec{q}) = \vec{0}$.

This concludes the computation for $\vec{\mathbf{Y}}_{lm} = \vec{Y}_{lm}$ and $\vec{\mathbf{Y}}_{l'm'} \in \{\vec{Y}_{l'm'}, \vec{\Psi}_{l'm'}, \vec{\Phi}_{l'm'}\}$. $\square_{(1)}$

(2) $\vec{\mathbf{Y}}_{lm} = \vec{\Psi}_{lm}$ **and** $\vec{\mathbf{Y}}_{l'm'} \in \{\vec{\Psi}_{l'm'}, \vec{\Phi}_{l'm'}\}$

Now we fix $\vec{\mathbf{Y}}_{lm}$ to be the first *tangential vector spherical harmonic* $\vec{\mathbf{Y}}_{lm} = \vec{\Psi}_{lm}$ and consider the two possibilities $\vec{\mathbf{Y}}_{l'm'} = \vec{\Psi}_{l'm'}$ and $\vec{\mathbf{Y}}_{l'm'} = \vec{\Phi}_{l'm'}$ one after the other. Since in every of the two cases both spherical harmonics carry a derivative, we can no longer suppress one of the momentum integrals.

(a) $\vec{\mathbf{Y}}_{l'm'} = \vec{\Psi}_{l'm'}$

Inserting the definitions of $\vec{\Psi}_{lm}$ and $\vec{\Psi}_{l'm'}$ yields

$$\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \int_{S^2} \mathrm{d}\Omega_\xi \; \vec{\Psi}_{lm}\cdot\vec{\Psi}_{l'm'} \mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} =$$
$$= \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)|\vec{q}| \big(\mathrm{grad}_{\vec{p}} Y_{lm}\cdot \mathrm{grad}_{\vec{q}} Y_{l'm'} \big) j_{0,1}(k_\pm r)$$

Integrating by parts with respect to $\vec{q}$ gives

$$\cdots = \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q} \; \Big[\mathrm{div}_{\vec{q}} \Big(k(|\vec{q}|)|\vec{q}| Y_{l'm'} j_{0,1}(k_\pm r)\, \mathrm{grad}_{\vec{p}} Y_{lm} \Big) - Y_{l'm'} \mathrm{div}_{\vec{q}} \Big(k(|\vec{q}|)|\vec{q}| j_{0,1}(k_\pm r)\, \mathrm{grad}_{\vec{p}} Y_{lm} \Big) \Big]$$

Rewriting the first term using the divergence theorem and carrying out the divergence in the second term results in

$$\cdots = \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \lim_{|\vec{q}|\to\infty} \left[k(|\vec{q}|)|\vec{q}|^2 \int_{S^2} \mathrm{d}\Omega_q \; Y_{l'm'} j_{0,1}(k_\pm r)\vec{q}\cdot \mathrm{grad}_{\vec{p}} Y_{lm} \right]$$
$$- \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{l'm'}\, \mathrm{grad}_{\vec{p}} Y_{lm} \cdot \left[\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|} \Big[k(|\vec{q}|)|\vec{q}| \Big] \frac{\vec{q}}{|\vec{q}|} j_{0,1}(k_\pm r) + k(|\vec{q}|)|\vec{q}|\, \mathrm{grad}_{\vec{q}} j_{0,1}(k_\pm r) \right]$$

To get rid of the derivative of $k(|\vec{q}|)$, we integrate the respective term by parts with respect to $|\vec{q}|$. Taking into account that the boundary term at $|\vec{q}| = 0$ vanishes due to $k \in C^1(\mathbb{R}_0^+, \mathbb{R})$, we obtain

$$\cdots = \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \lim_{|\vec{q}|\to\infty} \left[k(|\vec{q}|)|\vec{q}|^2 \int_{S^2} \mathrm{d}\Omega_q \; Y_{l'm'} j_{0,1}(k_\pm r)\vec{q}\cdot \mathrm{grad}_{\vec{p}} Y_{lm} \right]$$

$$- \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \lim_{|\vec{q}|\to\infty} \left[k(|\vec{q}|)|\vec{q}|^2 \int_{S^2} \mathrm{d}\Omega_q\; Y_{l'm'}\vec{q}\cdot \mathrm{grad}_{\vec{p}} Y_{lm} j_{0,1}(k_\pm r) \right]$$
$$+ \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \int_0^\infty \mathrm{d}|\vec{q}|\; k(|\vec{q}|)|\vec{q}| \int_{S^2} \mathrm{d}\Omega_q\; Y_{l'm'} \frac{\mathrm{d}}{\mathrm{d}|\vec{q}|} \left[|\vec{q}|\vec{q}\cdot \mathrm{grad}_{\vec{p}} Y_{lm} j_{0,1}(k_\pm r) \right]$$
$$- \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} |\vec{q}|\, \mathrm{grad}_{\vec{p}} Y_{lm}\cdot \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)$$

where the first two terms add up to zero. Next, we have to eliminate the gradients of Y_{lm}. To this end we integrate by parts with respect to $\vec{p}$ and thus find

$$\cdots = \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} \frac{1}{|\vec{q}|} \frac{\mathrm{d}}{\mathrm{d}|\vec{q}|} \Bigg[|\vec{q}| \Big[\mathrm{div}_{\vec{p}} \Big(h(|\vec{p}|)|\vec{p}| Y_{lm} j_{0,1}(k_\pm r)\vec{q} \Big) - Y_{lm} \mathrm{div}_{\vec{p}} \Big(h(|\vec{p}|)|\vec{p}| j_{0,1}(k_\pm r)\vec{q} \Big) \Big] \Bigg]$$
$$- \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} |\vec{q}| \Big[\mathrm{div}_{\vec{p}} \Big(h(|\vec{p}|)|\vec{p}| Y_{lm}\, \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) \Big) - Y_{lm} \mathrm{div}_{\vec{p}} \Big(h(|\vec{p}|)|\vec{p}|\, \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) \Big) \Big]$$

Repeating the above procedure, namely rewriting the first and third line using the divergence theorem and computing the remaining divergences in the second and fourth line, results in

$$\cdots = \lim_{|\vec{p}|\to\infty} \left[h(|\vec{p}|)|\vec{p}|^2 \int_{S^2} \mathrm{d}\Omega_p\; Y_{lm} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} \frac{1}{|\vec{q}|} \frac{\mathrm{d}}{\mathrm{d}|\vec{q}|} \Big[|\vec{q}| j_{0,1}(k_\pm r)(\vec{q}\cdot\vec{p}) \Big] \right]$$
$$- \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; Y_{lm} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} \frac{1}{|\vec{q}|} \frac{\mathrm{d}}{\mathrm{d}|\vec{q}|} \Big[|\vec{q}|\vec{q}\cdot \mathrm{grad}_{\vec{p}} \Big(h(|\vec{p}|)|\vec{p}| j_{0,1}(k_\pm r) \Big) \Big]$$
$$- \lim_{|\vec{p}|\to\infty} \left[h(|\vec{p}|)|\vec{p}|^2 \int_{S^2} \mathrm{d}\Omega_p\; Y_{lm} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} |\vec{q}|\vec{p}\cdot \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) \right]$$
$$+ \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; Y_{lm} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} |\vec{q}| \mathrm{div}_{\vec{p}} \Big(h(|\vec{p}|)|\vec{p}|\, \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) \Big)$$

At this point we have to compute the gradient with respect to $\vec{p}$ and divergence with respect to $\vec{q}$ in the second and fourth term, respectively. We obtain

$$\vec{q}\cdot \mathrm{grad}_{\vec{p}} \Big(h(|\vec{p}|)|\vec{p}| j_{0,1}(k_\pm r) \Big) = \frac{\big(h(|\vec{p}|)|\vec{p}| \big)'}{|\vec{p}|} (\vec{q}\cdot\vec{p}) j_{0,1}(k_\pm r) + h(|\vec{p}|)|\vec{p}|\vec{q}\cdot \mathrm{grad}_{\vec{p}}\, j_{0,1}(k_\pm r)$$
$$\mathrm{div}_{\vec{p}} \Big(h(|\vec{p}|)|\vec{p}|\, \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) \Big) = \frac{\big(h(|\vec{p}|)|\vec{p}| \big)'}{|\vec{p}|} \vec{p}\cdot \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) + h(|\vec{p}|)|\vec{p}| \mathrm{div}_{\vec{p}}\, \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)$$

Inserting this yields

$$\cdots = \lim_{|\vec{p}|\to\infty} \left[h(|\vec{p}|)|\vec{p}|^2 \int_{S^2} \mathrm{d}\Omega_p\; Y_{lm} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} \frac{1}{|\vec{q}|} \frac{\mathrm{d}}{\mathrm{d}|\vec{q}|} \Big[|\vec{q}| j_{0,1}(k_\pm r)(\vec{q}\cdot\vec{p}) \Big] \right]$$
$$- \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; Y_{lm} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} \frac{1}{|\vec{p}||\vec{q}|} \frac{\mathrm{d}}{\mathrm{d}|\vec{q}|} \Bigg[|\vec{q}| \frac{\mathrm{d}}{\mathrm{d}|\vec{p}|} \Big[h(|\vec{p}|)|\vec{p}| \Big] (\vec{q}\cdot\vec{p}) j_{0,1}(k_\pm r) + |\vec{p}||\vec{q}| h(|\vec{p}|)|\vec{p}|\vec{q}\cdot \mathrm{grad}_{\vec{p}}\, j_{0,1}(k_\pm r) \Bigg]$$
$$- \lim_{|\vec{p}|\to\infty} \left[h(|\vec{p}|)|\vec{p}|^2 \int_{S^2} \mathrm{d}\Omega_p\; Y_{lm} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} |\vec{q}|\vec{p}\cdot \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) \right]$$

$$+\int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; Y_{lm} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} \left[\frac{|\vec{q}|}{|\vec{p}|}\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\Big[h(|\vec{p}|)|\vec{p}|\Big]\vec{p}\cdot \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) + |\vec{q}| h(|\vec{p}|)|\vec{p}|\mathrm{div}_{\vec{p}}\,\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)\right]$$

To cancel the boundary terms, we have to integrate by parts with respect to $|\vec{p}|$ in the second and fifth line and thus obtain

$$\begin{aligned}
\cdots = &\lim_{|\vec{p}|\to\infty}\left[h(|\vec{p}|)|\vec{p}|^2 \int\limits_{S^2} \mathrm{d}\Omega_p\; Y_{lm} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} \frac{1}{|\vec{q}|}\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\Big[|\vec{q}| j_{0,1}(k_\pm r)(\vec{q}\cdot\vec{p})\Big]\right] \\
&- \lim_{|\vec{p}|\to\infty}\left[h(|\vec{p}|)|\vec{p}|^2 \int\limits_{S^2} \mathrm{d}\Omega_p\; Y_{lm} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} \frac{1}{|\vec{q}|}\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\Big[|\vec{q}|(\vec{q}\cdot\vec{p}) j_{0,1}(k_\pm r)\Big]\right] \\
&+ \int\limits_0^\infty \mathrm{d}|\vec{p}| \int\limits_{S^2} \mathrm{d}\Omega_p\; Y_{lm} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} \frac{1}{|\vec{q}|}\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[|\vec{q}| h(|\vec{p}|)|\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\Big[|\vec{p}|(\vec{q}\cdot\vec{p}) j_{0,1}(k_\pm r)\Big]\right] \\
&- \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; Y_{lm} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} \frac{1}{|\vec{q}|}\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\Big[|\vec{q}| h(|\vec{p}|)|\vec{p}|\vec{q}\cdot \mathrm{grad}_{\vec{p}}\, j_{0,1}(k_\pm r)\Big] \\
&- \lim_{|\vec{p}|\to\infty}\left[h(|\vec{p}|)|\vec{p}|^2 \int\limits_{S^2} \mathrm{d}\Omega_p\; Y_{lm} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} |\vec{q}|\vec{p}\cdot \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)\right] \\
&+ \lim_{|\vec{p}|\to\infty}\left[h(|\vec{p}|)|\vec{p}|^2 \int\limits_{S^2} \mathrm{d}\Omega_p\; Y_{lm} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} |\vec{q}|\vec{p}\cdot \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)\right] \\
&- \int\limits_0^\infty \mathrm{d}|\vec{p}|\; Y_{lm} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} |\vec{q}| h(|\vec{p}|)|\vec{p}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\Big[|\vec{p}|\vec{p}\cdot \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)\Big] \\
&+ \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) Y_{lm} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} |\vec{p}||\vec{q}|\mathrm{div}_{\vec{p}}\,\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)
\end{aligned}$$

Cancelling the boundary terms and combining the remaining terms we are left with

$$\begin{aligned}
\cdots = \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) Y_{lm} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} \Bigg[&\frac{1}{|\vec{p}||\vec{q}|}\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\left[|\vec{q}|\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\Big[|\vec{p}|(\vec{q}\cdot\vec{p}) j_{0,1}(k_\pm r)\Big]\right] \\
&- \frac{|\vec{p}|}{|\vec{q}|}\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\Big[|\vec{q}|\vec{q}\cdot \mathrm{grad}_{\vec{p}}\, j_{0,1}(k_\pm r)\Big] - \frac{|\vec{q}|}{|\vec{p}|}\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\Big[|\vec{p}|\vec{p}\cdot \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)\Big] \\
&+ |\vec{p}||\vec{q}|\mathrm{div}_{\vec{p}}\,\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)\Bigg]
\end{aligned}$$

Making use of the result in Auxiliary Calculation C.1.7 we end up with

$$\ldots \overset{\text{(C.27)}}{=} \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{lm} Y_{l'm'} \sum_{\substack{n=-1\\ n \text{ odd}}}^{5} \begin{cases} \overset{*}{\mathfrak{m}}{}^{(n)}_{\vec{\Psi}\vec{\Psi}'} j_{0,n}(k_+ r) \\ \overset{*}{\mathfrak{m}}{}^{(n)}_{\vec{\Psi}\vec{\Psi}'} j_{0,n}(k_- r) \end{cases} \tag{C.56}$$

where

$$\begin{Bmatrix} \overset{*}{\mathfrak{m}}{}^{(-1)}_{\vec{\Psi}\vec{\Psi}'} \\ \overset{*}{\mathfrak{n}}{}^{(-1)}_{\vec{\Psi}\vec{\Psi}'} \end{Bmatrix} = \begin{Bmatrix} +1 \\ -1 \end{Bmatrix} \frac{1}{2|\vec{p}||\vec{q}|r^2}\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]^2 \tag{C.56a}$$

$$\begin{Bmatrix} \overset{*}{\mathfrak{m}}{}^{(1)}_{\vec{\Psi}\vec{\Psi}'} \\ \overset{*}{\mathfrak{n}}{}^{(1)}_{\vec{\Psi}\vec{\Psi}'} \end{Bmatrix} = \begin{Bmatrix} -1 \\ +1 \end{Bmatrix} \frac{|\vec{p}|^2 + |\vec{q}|^2}{|\vec{p}||\vec{q}|}\left[2 + \frac{3r}{4}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.56b}$$

$$\begin{Bmatrix} \overset{*}{\mathfrak{m}}^{(3)}_{\vec{\Psi}\vec{\Psi}'} \\ \overset{*}{\mathfrak{n}}^{(3)}_{\vec{\Psi}\vec{\Psi}'} \end{Bmatrix} = \begin{Bmatrix} +1 \\ -1 \end{Bmatrix} \frac{(|\vec{p}|^2 - |\vec{q}|^2)^2}{|\vec{p}||\vec{q}|} r^2 \left[1 + \frac{2(|\vec{p}|^4 + |\vec{q}|^4) + (|\vec{p}|^2 + |\vec{q}|^2)^2}{2(|\vec{p}|^2 - |\vec{q}|^2)^2}\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\right]\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.56c}$$

$$\begin{Bmatrix} \overset{*}{\mathfrak{m}}^{(5)}_{\vec{\Psi}\vec{\Psi}'} \\ \overset{*}{\mathfrak{n}}^{(5)}_{\vec{\Psi}\vec{\Psi}'} \end{Bmatrix} = \begin{Bmatrix} -1 \\ +1 \end{Bmatrix} \frac{(|\vec{p}|^2 + |\vec{q}|^2)(|\vec{p}|^2 - |\vec{q}|^2)^2}{2|\vec{p}||\vec{q}|} r^4 \left[2 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right]\left[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right] \tag{C.56d}$$

(b) $\tilde{\mathbf{Y}}_{lm} = \vec{\Psi}$ and $\vec{\mathbf{Y}}_{l'm'} = \vec{\Phi}_{l'm'}$

Inserting the definitions of $\vec{\Psi}_{lm}$ and $\vec{\Phi}_{l'm'}$ yields

$$\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \int_{S^2} \mathrm{d}\Omega_\xi\; \vec{\Psi}_{lm} \cdot \vec{\Phi}_{l'm'} \mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} =$$
$$= \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)\, \mathrm{grad}_{\vec{p}} Y_{lm} \cdot \big(\vec{q} \times \mathrm{grad}_{\vec{q}} Y_{l'm'}\big) j_{0,1}(k_\pm r)$$
$$= \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)\big(\mathrm{grad}_{\vec{p}} Y_{lm} \times \vec{q}\big) \cdot \mathrm{grad}_{\vec{q}} Y_{l'm'} j_{0,1}(k_\pm r)$$

where we exploited the cyclicity of the triple product in the last equality. Integrating by parts with respect to $\vec{q}$ yields

$$\cdots = \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; \Big[\mathrm{div}_{\vec{q}}\Big(k(|\vec{q}|)|\vec{q}|Y_{l'm'} j_{0,1}(k_\pm r)\, \mathrm{grad}_{\vec{p}} Y_{lm} \times \vec{q}\Big) - Y_{l'm'}\mathrm{div}_{\vec{q}}\Big(k(|\vec{q}|)|\vec{q}| j_{0,1}(k_\pm r)\, \mathrm{grad}_{\vec{p}} Y_{lm} \times \vec{q}\Big)\Big]$$

Rewriting the first term using the divergence theorem and computing the divergence in the second term using $\mathrm{div}_{\vec{q}}\big(\mathrm{grad}_{\vec{p}} Y_{lm} \times \vec{q}\big) = \vec{q} \cdot \mathrm{curl}_{\vec{q}}\, \mathrm{grad}_{\vec{p}} Y_{lm} - \mathrm{grad}_{\vec{p}} Y_{lm} \cdot \mathrm{curl}_{\vec{q}} \vec{q} = \vec{0}$ results in

$$\cdots = \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \lim_{|\vec{q}|\to\infty} \Big[k(|\vec{q}|)|\vec{q}|^2 \int_{S^2} \mathrm{d}\Omega_q\; Y_{l'm'} j_{0,1}(k_\pm r) \vec{q} \cdot \big(\mathrm{grad}_{\vec{p}} Y_{lm} \times \vec{q}\big)\Big]$$
$$- \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{l'm'}\big(\mathrm{grad}_{\vec{p}} Y_{lm} \times \vec{q}\big) \cdot \mathrm{grad}_{\vec{q}}\big(k(|\vec{q}|)|\vec{q}| j_{0,1}(k_\pm r)\big)$$

By exploiting the cyclicity of the triple product once more and using $\vec{q} \times \vec{q} = \vec{0}$, the first term vanishes identically. Carrying out the gradient with respect to $\vec{q}$ in the second term turns the expression into

$$\cdots = -\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{l'm'}\big(\mathrm{grad}_{\vec{p}} Y_{lm} \times \vec{q}\big) \cdot \left[\frac{\mathrm{d}}{\mathrm{d}|\vec{q}|}\Big[k(|\vec{q}|)|\vec{q}|\Big] \frac{\vec{q}}{|\vec{q}|} j_{0,1}(k_\pm r) + k(|\vec{q}|)|\vec{q}|\, \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)\right]$$

Using the same reasoning as above, the term containing the derivative of $k(|\vec{q}|)$ vanishes. Using the cyclicity of the triple product the remaining term can be rewritten as follows

$$\cdots = -\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}| \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)|\vec{q}| Y_{l'm'}\, \mathrm{grad}_{\vec{p}} Y_{lm} \cdot \big(\vec{q} \times \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)\big)$$

In order to get rid of the gradient of Y_{lm} we integrate by parts with respect to $\vec{p}$ and thus find

$$\cdots = -\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)|\vec{q}| Y_{l'm'} \Big[\mathrm{div}_{\vec{p}}\Big(h(|\vec{p}|)|\vec{p}| Y_{lm}\big(\vec{q} \times \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)\big)\Big)$$

$$- Y_{lm}\mathrm{div}_{\vec{p}}\Big(h(|\vec{p}|)|\vec{p}|\big(\vec{q}\times \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)\big)\Big)\Big]$$

Rewriting the first term using the divergence theorem and carrying out the divergence in the second term using $\mathrm{div}_{\vec{p}}\left(\vec{q}\times \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)\right) = \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)\cdot \mathrm{curl}_{\vec{p}}\,\vec{q} - \vec{q}\cdot \mathrm{curl}_{\vec{p}}\, \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) = -\vec{q}\cdot(\mathrm{curl}_{\vec{p}}\, \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r))$, the expression becomes

$$\cdots = -\lim_{|\vec{p}|\to\infty}\Big[h(|\vec{p}|)|\vec{p}|^2 \int_{S^2} \mathrm{d}\Omega_p\, Y_{lm} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)|\vec{q}|Y_{l'm'}\big(\vec{q}\times \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)\big)\cdot\vec{p}\Big]$$
$$+ \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|)|\vec{p}|Y_{lm} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)|\vec{q}|Y_{l'm'}\vec{q}\cdot \mathrm{curl}_{\vec{p}}\, \mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r) \tag{C.57}$$

Recalling form (C.2a) that $\mathrm{grad}_{\vec{q}}\, j_{0,1}(k_\pm r)\big) \propto (\vec{p}\pm\vec{q})$, the first term vanishes as a consequence of the cyclicity of the triple product and the properties of the cross product. Due to the fact that according to (C.3b) also the integrand of the second term vanishes, we find that the whole expression vanishes. This means that we have $\overset{*}{\mathfrak{m}}{}^{(n)}_{\vec{\Psi}\vec{\Phi}'} = 0 = \overset{*}{\mathfrak{n}}{}^{(n)}_{\vec{\Psi}\vec{\Phi}'}$ for all $n\in\mathbb{Z}$.

This concludes the computation for $\vec{\mathbf{Y}}_{lm} = \vec{\Psi}_{lm}$ and $\vec{\mathbf{Y}}_{l'm'} \in \{\vec{\Psi}_{l'm'}, \vec{\Phi}_{l'm'}\}$. $\square_{(2)}$

(3) $\vec{\mathbf{Y}}_{lm} = \vec{\Phi}_{lm}$ **and** $\vec{\mathbf{Y}}_{l'm'} = \vec{\Phi}_{l'm'}$

Finally, we fix $\vec{\mathbf{Y}}_{lm}$ to be the second tangential vector spherical harmonic $\vec{\mathbf{Y}}_{lm} = \vec{\Phi}_{lm}$ and consider the only remaining case $\vec{\mathbf{Y}}_{l'm'} = \vec{\Phi}_{l'm'}$. Just as before, again both momentum integrals are needed. Inserting the definitions of $\vec{\Phi}_{lm}$ and $\vec{\Phi}_{l'm'}$ yields

$$\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \int_{S^2} \mathrm{d}\Omega_\xi\; \vec{\Phi}_{lm}(\theta_p,\varphi_p)\cdot\vec{\Phi}_{l'm'}(\theta_q,\varphi_q)\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} =$$
$$= \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)\big(\vec{p}\times \mathrm{grad}_{\vec{p}}\, Y_{lm}\big)\cdot\big(\vec{q}\times \mathrm{grad}_{\vec{q}}\, Y_{l'm'}\big) j_{0,1}(k_\pm r)$$
$$= \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|)\Big[(\vec{p}\cdot\vec{q})\big(\mathrm{grad}_{\vec{p}}\, Y_{lm}\cdot \mathrm{grad}_{\vec{q}}\, Y_{l'm'}\big) - \big(\vec{q}\cdot \mathrm{grad}_{\vec{p}}\, Y_{lm}\big)\big(\vec{p}\cdot \mathrm{grad}_{\vec{q}}\, Y_{l'm'}\big)\Big] j_{0,1}(k_\pm r)$$

where in the last equality we employed the identity $(\vec{v}_1\times\vec{v}_2)\cdot(\vec{v}_3\times\vec{v}_4) = (\vec{v}_1\cdot\vec{v}_3)(\vec{v}_2\cdot\vec{v}_4) - (\vec{v}_2\cdot\vec{v}_3)(\vec{v}_1\cdot\vec{v}_4)$ to rewrite the scalar product of two cross products. Integrating by parts with respect to $\vec{q}$ yields

$$\cdots = \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; \Big[\mathrm{div}_{\vec{q}}\Big(k(|\vec{q}|)Y_{l'm'}(\vec{p}\cdot\vec{q})\, \mathrm{grad}_{\vec{p}}\, Y_{lm} j_{0,1}(k_\pm r)\Big)$$
$$- Y_{l'm'}\mathrm{div}_{\vec{q}}\Big(k(|\vec{q}|)(\vec{p}\cdot\vec{q})\, \mathrm{grad}_{\vec{p}}\, Y_{lm} j_{0,1}(k_\pm r)\Big)$$
$$- \mathrm{div}_{\vec{q}}\Big(k(|\vec{q}|)Y_{l'm'}\big(\vec{q}\cdot \mathrm{grad}_{\vec{p}}\, Y_{lm}\big)\vec{p} j_{0,1}(k_\pm r)\Big)$$
$$+ Y_{l'm'}\mathrm{div}_{\vec{q}}\Big(k(|\vec{q}|)\big(\vec{q}\cdot \mathrm{grad}_{\vec{p}}\, Y_{lm}\big)\vec{p} j_{0,1}(k_\pm r)\Big)\Big]$$

By applying the divergence theorem, the first and third term can be converted into surface integrals, while the divergences with respect to $\vec{q}$ in the second and fourth term can be rewritten as gradients with respect to $\vec{q}$. Rearranging terms gives

$$\cdots = \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \lim_{|\vec{q}|\to\infty}\Big[k(|\vec{q}|)|\vec{q}|^2 \int_{S^2} \mathrm{d}\Omega_q\; Y_{l'm'} j_{0,1}(k_\pm r)\times$$

$$\times \Big[(\vec{p}\cdot\vec{q})\,\mathrm{grad}_{\vec{p}} Y_{lm} - \big(\vec{q}\cdot\mathrm{grad}_{\vec{p}} Y_{lm}\big)\vec{p}\Big]\cdot\frac{\vec{q}}{|\vec{q}|}\Big]$$

$$- \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{l'm'}\,\mathrm{grad}_{\vec{p}} Y_{lm}\cdot \mathrm{grad}_{\vec{q}}\Big(k(|\vec{q}|)(\vec{p}\cdot\vec{q})j_{0,1}(k_\pm r)\Big)$$

$$+ \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{l'm'}\vec{p}\cdot \mathrm{grad}_{\vec{q}}\Big(k(|\vec{q}|)\big(\vec{q}\cdot\mathrm{grad}_{\vec{p}} Y_{lm}\big)j_{0,1}(k_\pm r)\Big)$$

As can be easily seen in this form, the difference in the integrand of the first term vanishes identically. In the last term, the gradient with respect to $\vec{q}$ can be rewritten as follows

$$\begin{aligned}
&\mathrm{grad}_{\vec{q}}\Big(k(|\vec{q}|)\big(\vec{q}\cdot\mathrm{grad}_{\vec{p}} Y_{lm}\big)j_{0,1}(k_\pm r)\Big) = \\
&= \mathrm{grad}_{\vec{q}}\big(k(|\vec{q}|)j_{0,1}(k_\pm r)\big)\big(\vec{q}\cdot\mathrm{grad}_{\vec{p}} Y_{lm}\big) + k(|\vec{q}|)j_{0,1}(k_\pm r)\,\mathrm{grad}_{\vec{q}}\big(\vec{q}\cdot\mathrm{grad}_{\vec{p}} Y_{lm}\big)\\
&= \mathrm{grad}_{\vec{q}}\big(k(|\vec{q}|)j_{0,1}(k_\pm r)\big)\big(\vec{q}\cdot\mathrm{grad}_{\vec{p}} Y_{lm}\big) + k(|\vec{q}|)j_{0,1}(k_\pm r)\,\mathrm{grad}_{\vec{p}} Y_{lm}
\end{aligned}$$

Upon scalar multiplication with $\vec{p}$, the second term vanishes for orthogonality reasons due to the fact that $\mathrm{grad}_{\vec{p}} Y_{lm}$ is tangential to S^2 while $\vec{p}$ is radial. Inserting the remaining term, we therefore end up with

$$\begin{aligned}
\cdots = &- \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{l'm'}\,\mathrm{grad}_{\vec{p}} Y_{lm}\cdot \mathrm{grad}_{\vec{q}}\Big(k(|\vec{q}|)(\vec{p}\cdot\vec{q})j_{0,1}(k_\pm r)\Big)\\
&+ \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{l'm'}\vec{p}\cdot \mathrm{grad}_{\vec{q}}\big(k(|\vec{q}|)j_{0,1}(k_\pm r)\big)\big(\vec{q}\cdot\mathrm{grad}_{\vec{p}} Y_{lm}\big)
\end{aligned}$$

Integrating by parts for a second time, but now with respect to $\vec{p}$, results in

$$\begin{aligned}
\cdots = &- \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{l'm'}\Big[\mathrm{div}_{\vec{p}}\Big[h(|\vec{p}|)Y_{lm}\,\mathrm{grad}_{\vec{q}}\Big(k(|\vec{q}|)(\vec{p}\cdot\vec{q})j_{0,1}(k_\pm r)\Big]\\
&\qquad - Y_{lm}\mathrm{div}_{\vec{p}}\Big[h(|\vec{p}|)\,\mathrm{grad}_{\vec{q}}\Big(k(|\vec{q}|)(\vec{p}\cdot\vec{q})j_{0,1}(k_\pm r)\Big)\Big]\Big]\\
&+ \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{l'm'}\Big[\mathrm{div}_{\vec{p}}\Big[h(|\vec{p}|)Y_{lm}\vec{q}\Big(\vec{p}\cdot\mathrm{grad}_{\vec{q}}\big(k(|\vec{q}|)j_{0,1}(k_\pm r)\big)\Big)\Big]\\
&\qquad - Y_{lm}\mathrm{div}_{\vec{p}}\Big[h(|\vec{p}|)\vec{q}\big(\vec{p}\cdot\mathrm{grad}_{\vec{q}}\big(k(|\vec{q}|)j_{0,1}(k_\pm r)\big)\big)\Big]\Big]
\end{aligned}$$

By applying the divergence theorem for a second time and rewriting divergences as gradients whenever possible, we arrive at

$$\begin{aligned}
\cdots = &- \lim_{|\vec{p}|\to\infty}\Big[h(|\vec{p}|)|\vec{p}|\int_{S^2}\mathrm{d}\Omega_p\; Y_{lm}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\; Y_{l'm'}\vec{p}\cdot\mathrm{grad}_{\vec{q}}\Big(k(|\vec{q}|)(\vec{p}\cdot\vec{q})j_{0,1}(k_\pm r)\Big)\Big]\\
&+ \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{l'm'}Y_{lm}\mathrm{div}_{\vec{p}}\Big(h(|\vec{p}|)\,\mathrm{grad}_{\vec{q}}\Big(k(|\vec{q}|)(\vec{p}\cdot\vec{q})j_{0,1}(k_\pm r)\Big)\\
&+ \lim_{|\vec{p}|\to\infty}\Big[h(|\vec{p}|)|\vec{p}|\int_{S^2}\mathrm{d}\Omega_p\; Y_{lm}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\; Y_{l'm'}(\vec{q}\cdot\vec{p})\Big(\vec{p}\cdot\mathrm{grad}_{\vec{q}}\big(k(|\vec{q}|)j_{0,1}(k_\pm r)\big)\Big)\Big]\\
&- \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{l'm'}Y_{lm}\vec{q}\cdot\mathrm{grad}_{\vec{p}}\Big(h(|\vec{p}|)\big(\vec{p}\cdot\mathrm{grad}_{\vec{q}}\big(k(|\vec{q}|)j_{0,1}(k_\pm r)\big)\big)\Big)
\end{aligned}$$

By combining the first and third term and using $\mathrm{grad}_{\vec{q}}(\vec{p}\cdot\vec{q}) = \vec{p}$ we obtain

$$\cdots = - \lim_{|\vec{p}|\to\infty}\Big[h(|\vec{p}|)|\vec{p}|^3\int_{S^2}\mathrm{d}\Omega_p\; Y_{lm}\int_{\mathbb{R}^3}\mathrm{d}^3\vec{q}\; Y_{l'm'}k(|\vec{q}|)j_{0,1}(k_\pm r)\Big]$$

$$+\int_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{lm} Y_{l'm'} \frac{1}{|\vec{p}||\vec{q}|} \Big[\mathrm{div}_{\vec{p}} \Big[h(|\vec{p}|) \,\mathrm{grad}_{\vec{q}} \Big(k(|\vec{q}|)(\vec{p}\cdot\vec{q}) j_{0,1}(k_\pm r) \Big) \Big] \\ - \vec{q}\cdot \mathrm{grad}_{\vec{p}} \Big[h(|\vec{p}|) \Big(\vec{p}\cdot \mathrm{grad}_{\vec{q}} \big(k(|\vec{q}|) j_{0,1}(k_\pm r) \big) \Big) \Big] \Big]$$

Making use of the result from Auxiliary Calculation C.1.8 gives

$$\begin{aligned} \ldots &\overset{(C.30)}{=} -\lim_{|\vec{p}|\to\infty} \Big[h(|\vec{p}|)|\vec{p}|^3 \int_{S^2} \mathrm{d}\Omega_p\; Y_{lm} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{l'm'} k(|\vec{q}|) j_{0,1}(k_\pm r) \Big] \\ &+ \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{lm} Y_{l'm'} h'(|\vec{p}|)|\vec{p}| j_{0,1}(k_\pm r) \\ &+ \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{lm} Y_{l'm'} \times \\ &\times \Big[\Big[3 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} \Big] j_{0,1}(k_\pm r) + (|\vec{p}|^2 - |\vec{q}|^2) r^2 \Big[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} \Big] j_{0,3}(k_\pm r) \Big] \end{aligned} \tag{C.58}$$

Integrating the term containing $h'(|\vec{p}|)$ by parts with respect to $|\vec{p}|$ gives

$$\begin{aligned} \cdots &= -\lim_{|\vec{p}|\to\infty} \Big[h(|\vec{p}|)|\vec{p}|^3 \int_{S^2} \mathrm{d}\Omega_p\; Y_{lm} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; Y_{l'm'} k(|\vec{q}|) j_{0,1}(k_\pm r) \Big] \\ &+ \lim_{|\vec{p}|\to\infty} \Big[h(|\vec{p}|)|\vec{p}|^3 \int_{S^2} \mathrm{d}\Omega_p\; Y_{lm} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} j_{0,1}(k_\pm r) \Big] \\ &- \int_0^\infty \mathrm{d}|\vec{p}| \int_{S^2} \mathrm{d}\Omega_p\; Y_{lm} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{l'm'} h(|\vec{p}|) \frac{\mathrm{d}}{\mathrm{d}|\vec{p}|} \Big[|\vec{p}|^3 j_{0,1}(k_\pm r) \Big] \\ &+ \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{lm} Y_{l'm'} \times \\ &\times \Big[\Big[3 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} \Big] j_{0,1}(k_\pm r) + (|\vec{p}|^2 - |\vec{q}|^2) r^2 \Big[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} \Big] j_{0,3}(k_\pm r) \Big] \end{aligned}$$

Cancelling the boundary terms yields

$$\begin{aligned} \ldots &\overset{(C.2d)}{=} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) Y_{lm} Y_{l'm'} \Big[-\frac{1}{|\vec{p}|^2} \frac{\mathrm{d}}{\mathrm{d}|\vec{p}|} \Big[|\vec{p}|^3 j_{0,1}(k_\pm r) \Big] + \\ &+ \Big[3 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} \Big] j_{0,1}(k_\pm r) + (|\vec{p}|^2 - |\vec{q}|^2) r^2 \Big[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} \Big] j_{0,3}(k_\pm r) \Big] \end{aligned}$$

Evaluating $\frac{\mathrm{d}}{\mathrm{d}|\vec{p}|}\Big[|\vec{p}|^3 j_{0,1}(k_\pm r)\Big]$ using (C.2d) gives

$$\begin{aligned} \frac{1}{|\vec{p}|^2} \frac{\mathrm{d}}{\mathrm{d}|\vec{p}|} \Big[|\vec{p}|^3 j_{0,1}(k_\pm r) \Big] &= \\ &= 3 j_{0,1}(k_\pm r) + |\vec{p}| \frac{\mathrm{d}}{\mathrm{d}|\vec{p}|} j_{0,1}(k_\pm r) \\ &\overset{(C.2d)}{=} 3 j_{0,1}(k_\pm r) + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} j_{0,n}(k_\pm r) + (|\vec{p}|^2 - |\vec{q}|^2) r^2 \Big[1 + \frac{r}{2}\frac{\mathrm{d}}{\mathrm{d}r} \Big] j_{0,n+2}(k_\pm r) \end{aligned}$$

which exactly cancels the second line in the above equation and thus makes the whole expression vanish. This means that $\overset{*}{\mathfrak{m}}{}^{(n)}_{\vec{\Phi}\vec{\Phi}'} = 0 = \overset{*}{\mathfrak{n}}{}^{(n)}_{\vec{\Phi}\vec{\Phi}'}$ for all $n \in \mathbb{Z}$.

This concludes the computation for $\vec{\mathbf{Y}}_{lm} = \vec{\Phi}_{lm}$ and $\vec{\mathbf{Y}}_{l'm'} = \vec{\Phi}_{l'm'}$. $\square_{(3)}$

Up to this point the we have only determined the entries of the operator-valued matrices $\overset{*}{\mathfrak{m}}^{(n)}$ and $\overset{*}{\mathfrak{n}}^{(n)}$ lying on or above the diagonal. By simultaneously interchanging the functions $h \leftrightarrow k$, the variables $\vec{p} \leftrightarrow \vec{q}$ and the parameters $(l,m) \leftrightarrow (l'm')$ the expression

$$\int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{p}\; h(|\vec{p}|) \int\limits_{\mathbb{R}^3} \mathrm{d}^3\vec{q}\; k(|\vec{q}|) \int\limits_{S^2} \mathrm{d}\Omega_\xi\; \vec{\mathbf{Y}}_{lm}(\theta_p,\varphi_p)\cdot\vec{\mathbf{Y}}_{l'm'}(\theta_q,\varphi_q)\mathrm{e}^{-\mathrm{i}(\vec{p}\pm\vec{q})\cdot\vec{\xi}} \tag{C.59}$$

remains unchanged except for an additional factor (± 1) appearing in the exponential. However, due to Proposition C.1.1 this factor disappears upon carrying out the position space angular integral. As a consequence, the entries of the matrices $\overset{*}{\mathfrak{m}}^{(n)}$ and $\overset{*}{\mathfrak{n}}^{(n)}$ below the diagonal can be found by interchanging $\vec{p} \leftrightarrow \vec{q}$ and $(l,m) \leftrightarrow (l'm')$ in the corresponding entries above the diagonal.

This concludes the proof. □

Having computed all the relevant integrals, we finally combine the derivative operators as deduced in Lemma C.2.1, Corollary C.2.2, Lemma C.3.1 and Lemma C.4.1, into (5×5)-matrices.

Definition C.4.2 (Matrix-Valued Derivative Operators)

For $n \in \{-1,1,3,5\}$ the (5×5)-matrix-valued derivative operators $\mathfrak{m}^{(n)}$, $\overset{*}{\mathfrak{m}}^{(n)}$ and $\mathfrak{n}^{(n)}$, $\overset{*}{\mathfrak{n}}^{(n)}$ are defined in terms of Hadamard products as

$$\mathfrak{m}^{(n)} = 4\pi\mathfrak{c}\odot\begin{pmatrix} \mathring{\mathfrak{m}}^{(n)} & \dot{\acute{\mathfrak{m}}}^{(n)\mathrm{T}} & \mathring{\mathfrak{m}}^{(n)} \\ \dot{\mathfrak{m}}^{(n)} & \ddot{\mathfrak{m}}^{(n)} & \dot{\mathfrak{m}}^{(n)} \\ \mathring{\mathfrak{m}}^{(n)} & \dot{\acute{\mathfrak{m}}}^{(n)\mathrm{T}} & \mathring{\mathfrak{m}}^{(n)} \end{pmatrix} \tag{C.60a}$$

$$\overset{*}{\mathfrak{m}}^{(n)} = 4\pi\begin{pmatrix} 0 & 0_{1\times 3} & 0 \\ 0_{3\times 1} & \overset{*}{\mathfrak{m}}^{(n)} & 0_{3\times 1} \\ 0 & 0_{1\times 3} & 0 \end{pmatrix} \tag{C.60b}$$

$$\mathfrak{n}^{(n)} = 4\pi\mathfrak{c}\odot\begin{pmatrix} \mathring{\mathfrak{n}}^{(n)} & \dot{\acute{\mathfrak{n}}}^{(n)\mathrm{T}} & \mathring{\mathfrak{n}}^{(n)} \\ \dot{\mathfrak{n}}^{(n)} & \ddot{\mathfrak{n}}^{(n)} & \dot{\mathfrak{n}}^{(n)} \\ \mathring{\mathfrak{n}}^{(n)} & \dot{\acute{\mathfrak{n}}}^{(n)\mathrm{T}} & \mathring{\mathfrak{n}}^{(n)} \end{pmatrix} \tag{C.60c}$$

$$\overset{*}{\mathfrak{n}}^{(n)} = 4\pi\begin{pmatrix} 0 & 0_{1\times 3} & 0 \\ 0_{3\times 1} & \overset{*}{\mathfrak{n}}^{(n)} & 0_{3\times 1} \\ 0 & 0_{1\times 3} & 0 \end{pmatrix} \tag{C.60d}$$

where the entries are the dimensionless, matrix-valued derivative operators from Lemma C.2.1, Lemma C.3.1 and Lemma C.4.1, respectively. The *circled entries* $\mathring{\mathfrak{m}}^{(n)}$ and $\mathring{\mathfrak{n}}^{(n)}$ are given by

$$\mathring{\mathfrak{m}}^{(n)} = \mathring{\mathfrak{n}}^{(n)} = \delta_{n1}$$

Likewise, the matrix-valued derivative operator $\mathfrak{k}^{(1)}$ is defined as

$$\mathfrak{k}^{(1)} = 4\pi\mathfrak{c}_{\mathfrak{k}}\odot\begin{pmatrix} 1 & 0_{1\times 3} & 0 \\ 0_{3\times 1} & D_{\dot{\mathfrak{k}}^{(1)}} & 0_{3\times 1} \\ 0 & 0_{1\times 3} & 1 \end{pmatrix} \tag{C.61}$$

where $D_{\dot{\mathfrak{k}}^{(1)}}$ denotes the (3×3)-matrix with the entries of $\dot{\mathfrak{k}}^{(1)}$ (see Corollary C.2.2) on its diagonal. Finally, the matrices $\mathfrak{c}$ and $\mathfrak{c}_{\mathfrak{k}}$ are given by

$$\mathfrak{c} = \begin{pmatrix} 1 & \frac{\mathrm{i}}{|\vec{q}|}\mathbb{1}_{1\times 3} & 1 \\ \frac{\mathrm{i}}{|\vec{p}|}\mathbb{1}_{3\times 1} & \frac{1}{|\vec{p}||\vec{q}|}\mathbb{1}_{3\times 3} & \frac{\mathrm{i}}{|\vec{p}|}\mathbb{1}_{3\times 1} \\ 1 & \frac{\mathrm{i}}{|\vec{q}|}\mathbb{1}_{1\times 3} & 1 \end{pmatrix} \quad \text{and} \quad \mathfrak{c}_{\mathfrak{k}} = \begin{pmatrix} 1 & 0_{1\times 3} & 0 \\ 0_{3\times 1} & \frac{\mathrm{i}}{|\vec{p}|}\mathbb{1}_{3\times 3} & 0_{3\times 1} \\ 0 & 0_{1\times 3} & 1 \end{pmatrix} \tag{C.62}$$

D

Momentum Space Angular Integration: Computation of Integrals $I_n^\pm(\alpha, \rho)$

Contents

In this appendix we derive closed-form expressions for the integrals $I_n^\pm(\alpha, \rho)$ appearing in the derivation of explicit formulas for the eigenvalues of the integral operators $T_n^\pm$ in Lemma 4.2.13.

Before we start, we briefly sketch our overall approach: To derive a closed-form expression for the functions $I_n^\pm(\alpha, \rho)$ for any $n \in \mathbb{Z}$, we start in Proposition D.1.3 by explicitly evaluating $I_n^\pm(\alpha, \rho)$ in the cases $n \in \{0, 1, 2, 3\}$. Subsequently, in Proposition D.2.1 we derive recursion relations for $n \geq 4$ (increasing power n in the denominator in (D.1)) and for $n \leq 0$ (decreasing power n in the denominator in (D.1)) which allows to recursively determine $I_n^\pm(\alpha, \rho)$ for any $n \in \mathbb{Z} \setminus \{0, 1, 2, 3\}$. Based on these relations, we afterwards derive closed-form expressions in the cases $n \geq 4$ and $n \leq 0$ which ultimately results in a closed-form expression for the functions $I_n^\pm(\alpha, \rho)$ in Lemma D.2.3.

D.1 Basic Definitions and Preparatory Propositions

To begin with, we give the definition of the functions $I_n^\pm$ and introduce auxiliary functions which will frequently appear throughout the rest of this appendix.

Definition D.1.1 (Functions $I_n^\pm(\alpha, \rho)$)

For any $n \in \mathbb{Z}$ the functions $I_n^\pm : \mathbb{R}_0^+ \times (-1, 1) \to \mathbb{R}$ are defined as

$$I_n^\pm(\alpha, \rho) := \int_{-1}^{1} \mathrm{d}x \; \frac{\sin\left(\alpha\sqrt{1 \pm \rho x}\right)}{\sqrt{1 \pm \rho x}^{\,n}} \tag{D.1}$$

Definition D.1.2 (Auxiliary Cosine and Sine Functions)

For any $n \in \mathbb{Z}$ the *auxiliary cosine and sine functions* $c_n, s_n : \mathbb{R}_0^+ \times (-1,1) \to \mathbb{R}$ are defined as

$$c_n(\alpha,\rho) = \frac{\cos(\alpha\sqrt{1+\rho})}{(1+\rho)^{n/2}} - \frac{\cos(\alpha\sqrt{1-\rho})}{(1-\rho)^{n/2}} \tag{D.2a}$$

$$s_n(\alpha,\rho) = \frac{\sin(\alpha\sqrt{1+\rho})}{(1+\rho)^{n/2}} - \frac{\sin(\alpha\sqrt{1-\rho})}{(1-\rho)^{n/2}} \tag{D.2b}$$

We now start with the actual derivations by first evaluating the functions $I_n^{\pm}$ for $n \in \{0,1,2,3\}$.

Proposition D.1.3 (Evaluation of the Functions $I_n^{\pm}(\alpha,\rho)$ for $n \in \{0,1,2,3\}$)

For $n \in \{0,1,2,3\}$ the functions $I_n^{\pm}$ introduced in Definition D.1.1 evaluate to

$$I_n^{\pm}(\alpha,\rho) = \frac{2}{\rho}\begin{cases} -\frac{c_{-1}(\alpha,\rho)}{\alpha} + \frac{s_0(\alpha,\rho)}{\alpha^2} & \text{for } n=0 \\ -\frac{c_0(\alpha,\rho)}{\alpha} & \text{for } n=1 \\ \mathrm{Si}(\alpha\sqrt{1+\rho}) - \mathrm{Si}(\alpha\sqrt{1-\rho}) & \text{for } n=2 \\ \alpha\Big[\mathrm{Ci}(\alpha\sqrt{1+\rho}) - \mathrm{Ci}(\alpha\sqrt{1-\rho})\Big] - s_1(\alpha,\rho) & \text{for } n=3 \end{cases} \tag{D.3}$$

where Ci and Si denote the usual cosine and sine integral functions while c_n and s_n are the auxiliary cosine and sine functions introduced above in Definition D.1.2.

Proof. In order to prove the claimed relations, we distinguish between the rather straightforward cases $n=0$ and $n=2$ on the one hand, and the slightly more involved cases $n=1$ and $n=3$ on the other hand.

(1) Evaluation of $I_n^{\pm}(\alpha,\rho)$ for $n=0$ and $n=2$
We start by considering the case $n=0$ and afterwards compute $I_n^{\pm}(\alpha,\rho)$ for $n=2$. Note that we treat the expressions where $\sin(\alpha\sqrt{1\pm x})$ in $I_n^{\pm}(\alpha,\rho)$ is replaced by $\cos(\alpha\sqrt{1\pm x})$ simultaneously.

(a) $I_n^{\pm}(\alpha,\rho)$ for $n=0$
By substituting $y=\alpha\sqrt{1\pm\rho x}$ in the expression for $I_0^{\pm}(\alpha,\rho)$ (and the analogous expression with sine replaced by cosine) we obtain

$$\int_{-1}^{1} \mathrm{d}x \begin{Bmatrix} \sin(\alpha\sqrt{1\pm\rho x}) \\ \cos(\alpha\sqrt{1\pm\rho x}) \end{Bmatrix} = \pm\frac{2}{\rho}\frac{1}{\alpha^2}\int_{\alpha\sqrt{1\mp\rho}}^{\alpha\sqrt{1\pm\rho}} \mathrm{d}y\; y \begin{Bmatrix} \sin(y) \\ \cos(y) \end{Bmatrix}$$

Integrating by parts leads to

$$\cdots = \pm\frac{2}{\rho}\frac{1}{\alpha^2}\left[-\int_{\alpha\sqrt{1\mp\rho}}^{\alpha\sqrt{1\pm\rho}} \mathrm{d}y \begin{Bmatrix} -\cos(y) \\ \sin(y) \end{Bmatrix} \right.$$

$$\left. + \alpha\begin{Bmatrix} -\sqrt{1\pm\rho}\cos(\alpha\sqrt{1\pm\rho}) + \sqrt{1\mp\rho}\cos(\alpha\sqrt{1\mp\rho}) \\ \sqrt{1\pm\rho}\sin(\alpha\sqrt{1\pm\rho}) - \sqrt{1\mp\rho}\sin(\alpha\sqrt{1\mp\rho}) \end{Bmatrix}\right]$$

Evaluating the remaining integral results in

$$\cdots = \pm\frac{2}{\rho}\frac{1}{\alpha^2}\left[\begin{Bmatrix}\sin(\alpha\sqrt{1\pm\rho}) - \sin(\alpha\sqrt{1\mp\rho})\\ \cos(\alpha\sqrt{1\pm\rho}) - \cos(\alpha\sqrt{1\mp\rho})\end{Bmatrix}\right.$$
$$\left. +\alpha\begin{Bmatrix}-\sqrt{1\pm\rho}\cos(\alpha\sqrt{1\pm\rho}) + \sqrt{1\mp\rho}\cos(\alpha\sqrt{1\mp\rho})\\ \sqrt{1\pm\rho}\sin(\alpha\sqrt{1\pm\rho}) - \sqrt{1\mp\rho}\sin(\alpha\sqrt{1\mp\rho})\end{Bmatrix}\right]$$

Taking the overall prefactor (±1) into account, we recognize that both cases $\pm$ lead to the same result, namely

$$\cdots = \frac{2}{\rho}\frac{1}{\alpha^2}\left[\begin{Bmatrix}\sin(\alpha\sqrt{1+\rho}) - \sin(\alpha\sqrt{1-\rho})\\ \cos(\alpha\sqrt{1+\rho}) - \cos(\alpha\sqrt{1-\rho})\end{Bmatrix}\right.$$
$$\left. +\alpha\begin{Bmatrix}-\sqrt{1+\rho}\cos(\alpha\sqrt{1+\rho}) + \sqrt{1-\rho}\cos(\alpha\sqrt{1-\rho})\\ \sqrt{1+\rho}\sin(\alpha\sqrt{1+\rho}) - \sqrt{1-\rho}\sin(\alpha\sqrt{1-\rho})\end{Bmatrix}\right]$$

Making use of the functions c_n, s_n introduced Definition D.1.2, the result can be displayed in the following compact form

$$\int_{-1}^{1} \mathrm{d}x \begin{Bmatrix}\sin(\alpha\sqrt{1\pm\rho x})\\ \cos(\alpha\sqrt{1\pm\rho x})\end{Bmatrix} = \frac{2}{\rho}\frac{1}{\alpha^2}\left[\begin{Bmatrix}s_0(\alpha,\rho)\\ c_0(\alpha,\rho)\end{Bmatrix} + \alpha\begin{Bmatrix}-c_{-1}(\alpha,\rho)\\ s_{-1}(\alpha,\rho)\end{Bmatrix}\right] \tag{D.4}$$

(b) $I_n^{\pm}(\alpha,\rho)$ for $n=2$

For the expression $I_2^{\pm}(\alpha,\rho)$ and the analogous expression with sine replaced by cosine, the computations are slightly different. Changing variables $y=\alpha\sqrt{1\pm\rho x}$ just as before, we obtain for $I_2^{\pm}(\alpha,\rho)$

$$\int_{-1}^{1} \mathrm{d}x\, \frac{1}{1\pm\rho x}\begin{Bmatrix}\sin(\alpha\sqrt{1\pm\rho x})\\ \cos(\alpha\sqrt{1\pm\rho x})\end{Bmatrix} = \pm\frac{2}{\rho}\int_{\alpha\sqrt{1\mp\rho}}^{\alpha\sqrt{1\pm\rho}} \mathrm{d}y\, \frac{1}{y}\begin{Bmatrix}\sin(y)\\ \cos(y)\end{Bmatrix}$$

At this point, the computations for the upper and lower case are slightly different: In the upper case we rewrite the integral as the difference of two integrals with domains $\left[0,\alpha\sqrt{1\pm\rho}\right]$ and $\left[0,\alpha\sqrt{1\mp\rho}\right]$ while in the lower case, however, we rewrite the integral as the difference of two integrals with domains $\left[\alpha\sqrt{1\mp\rho},\infty\right]$ and $\left[\alpha\sqrt{1\pm\rho},\infty\right]$. In this way we obtain

$$\cdots = \pm\frac{2}{\rho}\begin{Bmatrix}\int_0^{\alpha\sqrt{1\pm\rho}} \mathrm{d}y\, \frac{\sin(y)}{y} - \int_0^{\alpha\sqrt{1\mp\rho}} \mathrm{d}y\, \frac{\sin(y)}{y}\\ \int_{\alpha\sqrt{1\mp\rho}}^{\infty} \mathrm{d}y\, \frac{\cos(y)}{y} - \int_{\alpha\sqrt{1\pm\rho}}^{\infty} \mathrm{d}y\, \frac{\cos(y)}{y}\end{Bmatrix}$$

Identifying the remaining integrals as the sine and cosine integral functions $\mathrm{Si}(x) = \int_0^x \mathrm{d}y\, \sin(y)/y$ and $\mathrm{Ci}(x) = -\int_x^\infty \mathrm{d}y\, \cos(y)/y$, respectively, we finally end up with

$$\cdots = \pm\frac{2}{\rho}\begin{Bmatrix}\mathrm{Si}\big(\alpha\sqrt{1\pm\rho}\big) - \mathrm{Si}\big(\alpha\sqrt{1\mp\rho}\big)\\ \mathrm{Ci}\big(\alpha\sqrt{1\pm\rho}\big) - \mathrm{Ci}\big(\alpha\sqrt{1\mp\rho}\big)\end{Bmatrix}$$

Taking the prefactor (±1) into account, both cases $\pm$ again lead to the same result which reads

$$\int_{-1}^{1} \mathrm{d}x\, \frac{1}{1\pm\rho x}\begin{Bmatrix}\sin(\alpha\sqrt{1\pm\rho x})\\ \cos(\alpha\sqrt{1\pm\rho x})\end{Bmatrix} = \frac{2}{\rho}\begin{Bmatrix}\mathrm{Si}\big(\alpha\sqrt{1+\rho}\big) - \mathrm{Si}\big(\alpha\sqrt{1-\rho}\big)\\ \mathrm{Ci}\big(\alpha\sqrt{1+\rho}\big) - \mathrm{Ci}\big(\alpha\sqrt{1-\rho}\big)\end{Bmatrix} \tag{D.5}$$

(2) Evaluation of $I_n^{\pm}(\alpha,\rho)$ for $n=1$ and $n=3$
In order to derive the claimed expressions for $I_n^{\pm}(\alpha,\rho)$ in the cases $n=1$ and $n=3$, we make use of the identity

$$(1\pm\rho x)^{-\frac{n}{2}} = \pm\frac{2}{\rho}\frac{1}{(2-n)}\frac{\mathrm{d}}{\mathrm{d}x}(1\pm\rho x)^{-\frac{n}{2}+1} \tag{D.6}$$

which holds for $n\in\mathbb{Z}\setminus\{2\}$. Replacing the factor $(1\pm\rho x)^{-\frac{n}{2}}$ in the definition of $I_n^{\pm}(\alpha,\rho)$ by the above identity and integrating by parts yields

$$\begin{aligned}\int_{-1}^{1}\mathrm{d}x\ \frac{\sin\left(\alpha\sqrt{1\pm\rho x}\right)}{\sqrt{1\pm\rho x}^{\,n}} &\overset{\text{(D.6)}}{=} \pm\frac{2}{\rho}\frac{1}{(2-n)}\int_{-1}^{1}\mathrm{d}x\ \sin\left(\alpha\sqrt{1\pm\rho x}\right)\frac{\mathrm{d}}{\mathrm{d}x}(1\pm\rho x)^{-\frac{n}{2}+1}\\ &= \pm\frac{2}{\rho}\frac{1}{(2-n)}\Bigg[\mp\frac{\rho\alpha}{2}\int_{-1}^{1}\mathrm{d}x\ \cos\left(\alpha\sqrt{1\pm\rho x}\right)(1\pm\rho x)^{-\frac{n-1}{2}}\\ &\qquad + \left[\sin\left(\alpha\sqrt{1\pm\rho x}\right)(1\pm\rho x)^{-\frac{n}{2}+1}\right]\Bigg|_{-1}^{1}\Bigg]\end{aligned} \tag{D.7}$$

Evaluating this expression for $n=1$ and making use of the lower case in (D.4) yields

$$\begin{aligned}I_1^{\pm}(\alpha,\rho) &\overset{\text{(D.7)}}{=} \pm\frac{2}{\rho}\left[\mp\frac{\rho\alpha}{2}\int_{-1}^{1}\mathrm{d}x\ \cos\left(\alpha\sqrt{1\pm\rho x}\right) + \left[\sin\left(\alpha\sqrt{1\pm\rho x}\right)\sqrt{1\pm\rho x}\right]\Bigg|_{-1}^{1}\right]\\ &\overset{\text{(D.4)}}{=} -\frac{2}{\rho}\frac{c_0(\alpha,\rho)}{\alpha}\end{aligned} \tag{D.8}$$

Repeating the procedure for $n=3$ and making use of the lower case in (D.5) gives

$$\begin{aligned}I_3^{\pm}(\alpha,\rho) &\overset{\text{(D.7)}}{=} \mp\frac{2}{\rho}\left[\mp\frac{\rho\alpha}{2}\int_{-1}^{1}\mathrm{d}x\ \frac{\cos(\alpha\sqrt{1\pm\rho x})}{1\pm\rho x} + \left[\frac{\sin\left(\alpha\sqrt{1\pm\rho x}\right)}{\sqrt{1\pm\rho x}}\right]\Bigg|_{-1}^{1}\right]\\ &\overset{\text{(D.5)}}{=} \frac{2}{\rho}\alpha\left[\mathrm{Ci}(\alpha\sqrt{1+\rho}) - \mathrm{Ci}(\alpha\sqrt{1-\rho})\right] - \frac{2}{\rho}s_1(\alpha,\rho)\end{aligned} \tag{D.9}$$

This concludes the proof. □

D.2 Derivation of Recursion Relations

Having found explicit expressions for the functions $I_n^{\pm}$ in the cases $n\in\{0,1,2,3\}$, we now extend these results to arbitrary $n\in\mathbb{Z}$ by deriving recursion relations.

Proposition D.2.1 (Recursion Relations for $I_n^{\pm}(\alpha,\rho)$)

For $n\in\mathbb{Z}$ with $n\geq 4$ and $n\leq 0$, respectively, the functions $I_n^{\pm}(\alpha,\rho)$ satisfy the following recursion relations

$$I_n^{\pm}(\alpha,\rho) = \begin{cases} f_n(\alpha)I_{n-2}^{\pm}(\alpha,\rho) + g_n(\alpha,\rho) & \text{for } n\geq 4\\ k_n(\alpha)I_{n+2}^{\pm}(\alpha,\rho) + l_n(\alpha,\rho) & \text{for } n\leq 0\end{cases} \tag{D.10}$$

where the functions $f_n, k_n : \mathbb{R}_0^+ \to \mathbb{R}$ (for $n\geq 4$) and $g_n, l_n : \mathbb{R}_0^+\times(-1,1)\to\mathbb{R}$ are given by

$$f_n(\alpha) := -\frac{\alpha^2}{(2-n)(3-n)} \quad \text{and} \quad g_n(\alpha,\rho) := -\frac{2}{\rho}\left[\frac{\alpha c_{n-3}(\alpha,\rho)}{(2-n)(3-n)} - \frac{s_{n-2}(\alpha,\rho)}{(2-n)}\right] \tag{D.10a}$$

$$k_n(\alpha) := -\frac{n(n-1)}{\alpha^2} \quad \text{and} \quad \ell_n(\alpha,\rho) := -\frac{2}{\rho}\left[\frac{(n-1)s_n(\alpha,\rho)}{\alpha^2} + \frac{c_{n-1}(\alpha,\rho)}{\alpha}\right] \tag{D.10b}$$

Proof. To prove the stated recursion relations, we consider the two cases separately.

(1) Derivation of a recursion relation for $I_n^{\pm}(\alpha, \rho)$ with $n \geq 4$

In order to derive the claimed recursion relation for $I_n^{\pm}(\alpha, \rho)$ in the case $n \geq 4$, we will repeatedly make use of the identity

$$(1 \pm \rho x)^{-\frac{n}{2}} = \pm\frac{2}{\rho}\frac{1}{(2-n)}\frac{\mathrm{d}}{\mathrm{d}x}(1 \pm \rho x)^{-\frac{n}{2}+1} \tag{D.11}$$

which holds for $n \in \mathbb{Z} \setminus \{2\}$. Replacing the factor $(1 \pm \rho x)^{-\frac{n}{2}}$ in the definition of $I_n^{\pm}(\alpha, \rho)$ by the above identity and integrating by parts yields

$$\begin{aligned}
\int_{-1}^{1} \mathrm{d}x\ \frac{\sin\left(\alpha\sqrt{1\pm\rho x}\right)}{\sqrt{1\pm\rho x}^{\,n}} &\overset{\text{(D.11)}}{=} \pm\frac{2}{\rho}\frac{1}{(2-n)}\int_{-1}^{1} \mathrm{d}x\ \sin\left(\alpha\sqrt{1\pm\rho x}\right)\frac{\mathrm{d}}{\mathrm{d}x}(1\pm\rho x)^{-\frac{n}{2}+1} \\
&\overset{\text{I.b.p.}}{=} \pm\frac{2}{\rho}\frac{1}{(2-n)}\Bigg[\mp\frac{\rho\alpha}{2}\int_{-1}^{1}\mathrm{d}x\ \cos\left(\alpha\sqrt{1\pm\rho x}\right)(1\pm\rho x)^{-\frac{n-1}{2}} \\
&\qquad + \left[\sin\left(\alpha\sqrt{1\pm\rho x}\right)(1\pm\rho x)^{-\frac{n}{2}+1}\right]\Bigg|_{-1}^{1}\Bigg]
\end{aligned} \tag{D.12}$$

Rewriting the second factor in the remaining integral using the identity (D.11) (with the replacement $n \to n-1$ with thus holds for $n \in \mathbb{Z} \setminus \{3\}$) and integrating by parts for a second time results in

$$\begin{aligned}
\ldots &\overset{\text{(D.11)}}{=} \pm\frac{2}{\rho}\frac{1}{(2-n)}\Bigg[-\frac{\alpha}{(3-n)}\int_{-1}^{1}\mathrm{d}x\ \cos\left(\alpha\sqrt{1\pm\rho x}\right)\frac{\mathrm{d}}{\mathrm{d}x}(1\pm\rho x)^{-\frac{n-1}{2}+1} \\
&\qquad + \left[\sin\left(\alpha\sqrt{1\pm\rho x}\right)(1\pm\rho x)^{-\frac{n}{2}+1}\right]\Bigg|_{-1}^{1}\Bigg] \\
&\overset{\text{I.b.p.}}{=} \pm\frac{2}{\rho}\frac{1}{(2-n)}\Bigg[-\frac{\alpha}{(3-n)}\Bigg(\pm\frac{\rho\alpha}{2}\int_{-1}^{1}\mathrm{d}x\ \sin\left(\alpha\sqrt{1\pm\rho x}\right)(1\pm\rho x)^{-\frac{n-1}{2}+\frac{1}{2}} \\
&\qquad + \left[\cos\left(\alpha\sqrt{1\pm\rho x}\right)(1\pm\rho x)^{-\frac{n-1}{2}+1}\right]\Bigg|_{-1}^{1}\Bigg) \\
&\qquad + \left[\sin\left(\alpha\sqrt{1\pm\rho x}\right)(1\pm\rho x)^{-\frac{n}{2}+1}\right]\Bigg|_{-1}^{1}\Bigg]
\end{aligned}$$

Simplifying this expression by multiplying out and taking into account that for the second and third terms both cases $\pm$ lead to the same result, we obtain for $n \in \mathbb{Z}$ with $n \geq 4$ the following recursion relation

$$I_n^{\pm}(\alpha,\rho) = -\frac{\alpha^2 I_{n-2}^{\pm}(\alpha,\rho)}{(2-n)(3-n)} - \frac{2}{\rho}\frac{\alpha}{(2-n)(3-n)}\left[\frac{\cos\left(\alpha\sqrt{1+\rho}\right)}{\sqrt{1+\rho}^{\,n-3}} - \frac{\cos\left(\alpha\sqrt{1-\rho}\right)}{\sqrt{1-\rho}^{\,n-3}}\right]$$

$$+\frac{2}{\rho}\frac{1}{(2-n)}\left[\frac{\sin\left(\alpha\sqrt{1+\rho}\right)}{\sqrt{1+\rho}^{\,n-2}}-\frac{\sin\left(\alpha\sqrt{1-\rho}\right)}{\sqrt{1-\rho}^{\,n-2}}\right]$$

$$=-\frac{\alpha^2 I^{\pm}_{n-2}(\alpha,\rho)}{(2-n)(3-n)}-\frac{2}{\rho}\frac{\alpha c_{n-3}(\alpha,\rho)}{(2-n)(3-n)}+\frac{2}{\rho}\frac{s_{n-2}(\alpha,\rho)}{(2-n)} \tag{D.13}$$

where for the last equality we again used the definitions of $c_n(\alpha,\rho)$ and $s_n(\alpha,\rho)$ introduced in Definition D.1.2. By defining the functions

$$f_n(\alpha):=-\frac{\alpha^2}{(2-n)(3-n)} \qquad \text{and} \qquad g_n(\alpha,\rho):=-\frac{2}{\rho}\left[\frac{\alpha c_{n-3}(\alpha,\rho)}{(2-n)(3-n)}-\frac{s_{n-2}(\alpha,\rho)}{(2-n)}\right] \tag{D.14}$$

the recursion relation for $n\geq 4$ takes the schematic form

$$I^{\pm}_n(\alpha,\rho)\overset{(D.13)}{\underset{(D.14)}{=}}f_n(\alpha)I^{\pm}_{n-2}(\alpha,\rho)+g_n(\alpha,\rho) \tag{D.15}$$

(2) Derivation of a recursion relation for $I^{\pm}_n(\alpha,\rho)$ with $n\leq 0$

To derive the recursion relation for $n\leq 0$, we need the identities

$$\sin(\alpha\sqrt{1\pm\rho x})=\mp\frac{2}{\rho}\frac{\sqrt{1\pm\rho x}}{\alpha}\frac{\mathrm{d}}{\mathrm{d}x}\cos(\alpha\sqrt{1\pm\rho x}) \tag{D.16}$$

$$\cos(\alpha\sqrt{1\pm\rho x})=\pm\frac{2}{\rho}\frac{\sqrt{1\pm\rho x}}{\alpha}\frac{\mathrm{d}}{\mathrm{d}x}\sin(\alpha\sqrt{1\pm\rho x}) \tag{D.17}$$

Replacing the factor $\sin(\alpha\sqrt{1\pm\rho x})$ in the definition of $I^{\pm}_n(\alpha,\rho)$ using the first of the above identities and subsequently integrating by parts, we obtain for $n\leq 0$

$$\int_{-1}^{1}\mathrm{d}x\;\frac{\sin(\alpha\sqrt{1\pm\rho x})}{\sqrt{1\pm\rho x}^{\,n}}\overset{(D.16)}{=}\mp\frac{2}{\rho}\frac{1}{\alpha}\int_{-1}^{1}\mathrm{d}x\;\frac{1}{\sqrt{1\pm\rho x}^{\,n-1}}\frac{\mathrm{d}}{\mathrm{d}x}\cos(\alpha\sqrt{1\pm\rho x})$$

$$\overset{\text{I.b.p.}}{=}\mp\frac{2}{\rho}\frac{1}{\alpha}\left[\pm\frac{\rho}{2}(n-1)\int_{-1}^{1}\mathrm{d}x\;\frac{1}{\sqrt{1\pm\rho x}^{\,n+1}}\cos(\alpha\sqrt{1\pm\rho x})+\left[\frac{\cos(\alpha\sqrt{1\pm\rho x})}{\sqrt{1\pm\rho x}^{\,n-1}}\right]\Bigg|_{-1}^{1}\right]$$

Rewriting the second factor in the remaining integral using the second of the above identities and integrating by parts for a second time leads to

$$\ldots\overset{(D.17)}{=}\mp\frac{2}{\rho}\frac{1}{\alpha}\left[\frac{(n-1)}{\alpha}\int_{-1}^{1}\mathrm{d}x\;\frac{1}{\sqrt{1\pm\rho x}^{\,n}}\frac{\mathrm{d}}{\mathrm{d}x}\sin(\alpha\sqrt{1\pm\rho x})+\left[\frac{\cos(\alpha\sqrt{1\pm\rho x})}{\sqrt{1\pm\rho x}^{\,n-1}}\right]\Bigg|_{-1}^{1}\right]$$

$$\overset{\text{I.b.p.}}{=}\mp\frac{2}{\rho}\frac{1}{\alpha}\left[\frac{(n-1)}{\alpha}\left(\pm\frac{\rho}{2}n\int_{-1}^{1}\mathrm{d}x\;\frac{\sin(\alpha\sqrt{1\pm\rho x})}{\sqrt{1\pm\rho x}^{\,n+2}}+\left[\frac{\sin(\alpha\sqrt{1\pm\rho x})}{\sqrt{1\pm\rho x}^{\,n}}\right]\Bigg|_{-1}^{1}\right)\right.$$

$$\left.+\left[\frac{\cos(\alpha\sqrt{1\pm\rho x})}{\sqrt{1\pm\rho x}^{\,n-1}}\right]\Bigg|_{-1}^{1}\right]$$

Simplifying this expression by multiplying out and taking into account that for the second and third terms both cases $\pm$ lead to the same result, we obtain for $n\leq 0$ the following recursion relation

$$I^{\pm}_n(\alpha,\rho)=-\frac{n(n-1)}{\alpha^2}I^{\pm}_{n+2}(\alpha,\rho)-\frac{2}{\rho}\frac{(n-1)}{\alpha^2}\left[\frac{\sin(\alpha\sqrt{1+\rho})}{\sqrt{1+\rho}^{\,n}}-\frac{\sin(\alpha\sqrt{1-\rho})}{\sqrt{1-\rho}^{\,n}}\right]$$

$$-\frac{2}{\rho}\frac{1}{\alpha}\left[\frac{\cos(\alpha\sqrt{1+\rho})}{\sqrt{1+\rho}^{\,n-1}}-\frac{\cos(\alpha\sqrt{1-\rho})}{\sqrt{1-\rho}^{\,n-1}}\right]$$

$$= -\frac{n(n-1)}{\alpha^2} I_{n+2}^\pm(\alpha,\rho) - \frac{2}{\rho}\frac{(n-1)s_n(\alpha,\rho)}{\alpha^2} - \frac{2}{\rho}\frac{c_{n-1}(\alpha,\rho)}{\alpha} \tag{D.18}$$

where for the last equality we once more employed the definitions of $s_n(\alpha,\rho)$ and $c_n(\alpha,\rho)$ defined at the beginning. By Defining the functions

$$k_n(\alpha) := -\frac{n(n-1)}{\alpha^2} \qquad \text{and} \qquad \ell_n(\alpha,\rho) := -\frac{2}{\rho}\left[\frac{(n-1)s_n(\alpha,\rho)}{\alpha^2} + \frac{c_{n-1}(\alpha,\rho)}{\alpha}\right] \tag{D.19}$$

the recursion relation takes the schematic form

$$I_n^\pm(\alpha,\rho) = k_n(\alpha) I_{n+2}^\pm(\alpha,\rho) + \ell_n(\alpha,\rho) \tag{D.20}$$

Note that for $n=0$ this formula correctly reproduces

$$I_0^\pm(\alpha,\rho) = -\frac{2}{\rho}\left[-\frac{s_0(\alpha,\rho)}{\alpha^2} + \frac{c_{-1}(\alpha,\rho)}{\alpha}\right] \tag{D.21}$$

in accordance with (D.3) in Proposition D.1.3.

This concludes the proof. □

This proposition allows to recursively evaluate the functions $I_n^\pm$ for arbitrary $n \in \mathbb{Z}$. In order to arrive at an explicit formula for any $n \in \mathbb{Z}$, we make use of the above recursion relations to derive a closed-form expression.

Proposition D.2.2 (Closed-Form Expressions for $I_n^\pm$ for $n \in \mathbb{Z} \setminus \{0,1,2,3\}$)

Let $F_{N,n} : \mathbb{R}_0^+ \to \mathbb{R}$ and $G_{N,n} : \mathbb{R}_0^+ \times (-1,1) \to \mathbb{R}$ be functions defined as

$$F_{N,n}(\alpha) = \prod_{i=1}^{n} f_{N+2i}(\alpha) \tag{D.22a}$$

$$G_{N,n}(\alpha,\rho) = \sum_{i=0}^{n-1}\left(\prod_{j=0}^{i-1} f_{N+2(n-j)}(\alpha)\right) g_{N+2(n-i)}(\alpha,\rho) \tag{D.22b}$$

where f_n, g_n are the functions introduced in (D.10a). Then, provided that $I_n^\pm(\alpha,\rho)$ satisfies the recursion relation

$$I_n^\pm(\alpha,\rho) \overset{\text{(D.10)}}{=} f_n(\alpha) I_{n-2}^\pm(\alpha,\rho) + g_n(\alpha,\rho) \tag{D.22c}$$

for $n \geq 4$, the following closed-form relation holds

$$I_n^\pm(\alpha,\rho) = \begin{cases} F_{2,\frac{n-2}{2}}(\alpha) I_2^\pm(\alpha,\rho) + G_{2,\frac{n-2}{2}}(\alpha,\rho) & \text{for } n \geq 4 \wedge n \text{ even} \\ F_{3,\frac{n-3}{2}}(\alpha) I_3^\pm(\alpha,\rho) + G_{3,\frac{n-3}{2}}(\alpha,\rho) & \text{for } n \geq 5 \wedge n \text{ odd} \end{cases} \tag{D.22d}$$

Furthermore, let $K_{N,n} : \mathbb{R}_0^+ \to \mathbb{R}$ and $L_{N,n} : \mathbb{R}_0^+ \times (-1,1) \to \mathbb{R}$ be functions defined as

$$K_{N,n}(\alpha) := \prod_{i=1}^{n} k_{N-2i}(\alpha) \tag{D.23a}$$

$$L_{N,n}(\alpha,\rho) := \sum_{i=0}^{n-1}\left(\prod_{j=0}^{i-1} k_{N-2(n-j)}(\alpha)\right) \ell_{N-2(n-i)}(\alpha,\rho) \tag{D.23b}$$

where k_n, l_n are the functions introduced in (D.10b). Then, provided that $I_n^{\pm}(\alpha,\rho)$ satisfies the recursion relation

$$I_n^{\pm}(\alpha,\rho) \overset{\text{(D.10)}}{=} k_n(\alpha) I_{n+2}^{\pm}(\alpha,\rho) + l_n(\alpha,\rho) \tag{D.23c}$$

for $n \leq -1$, the following closed-form relation holds

$$I_n^{\pm}(\alpha,\rho) = \begin{cases} K_{0,-\frac{n}{2}}(\alpha) I_0^{\pm}(\alpha,\rho) + L_{0,-\frac{n}{2}}(\alpha,\rho) & n \leq -2 \wedge n \text{ even} \\ K_{1,\frac{1-n}{2}}(\alpha) I_1^{\pm}(\alpha,\rho) + L_{1,\frac{1-n}{2}}(\alpha,\rho) & n \leq -1 \wedge n \text{ odd} \end{cases} \tag{D.23d}$$

Proof. We consider the two cases, namely the closed-form expression for $n \geq 4$ (increasing power n in the denominator of the function $I_n^{\pm}$) and $n \leq 0$ (decreasing power n in the denominator of the function $I_n^{\pm}$), separately.

(1) Closed-Form Expression for $n \geq 4$

To prove the claimed relation, we demonstrate via a proof by induction on n that

$$I_{N+2n}^{\pm}(\alpha,\rho) = F_{N,n}(\alpha) I_N^{\pm}(\alpha,\rho) + G_{N,n}(\alpha,\rho) \tag{D.24}$$

holds for all $n \geq 1$ where $N \in \mathbb{N}_0$ is an arbitrary, but fixed natural number.

(a) Base Case $n = 1$

In the initial case, namely for $n = 1$, the claimed relations reduces to

$$\begin{aligned} I_{N+2}^{\pm}(\alpha,\rho) &= F_{N,1}(\alpha) I_N^{\pm}(\alpha,\rho) + G_{N,1}(\alpha,\rho) \\ &\overset{\text{(D.22a)}}{\underset{\text{(D.22b)}}{=}} \left(\prod_{i=1}^{1} f_{N+2i}(\alpha) \right) I_N^{\pm}(\alpha,\rho) + \sum_{i=0}^{1-1} \left(\prod_{j=0}^{i-1} f_{N+2(1-j)}(\alpha) \right) g_{N+2(1-i)}(\alpha,\rho) \\ &= f_{N+2}(\alpha) I_N^{\pm}(\alpha,\rho) + \left(\prod_{j=0}^{0-1} f_{N+2(1-j)}(\alpha) \right) g_{N+2}(\alpha,\rho) \\ &= f_{N+2}(\alpha) I_N^{\pm}(\alpha,\rho) + g_{N+2}(\alpha,\rho) \end{aligned} \tag{D.25}$$

which precisely is the given recursion relation (D.10) for n replaced by $N+2$. As we assumed $N \in \mathbb{N}_0$ this demonstrates that the claimed relation holds for $n = 1$.

(b) Inductive Step $n_0 \to n_0 + 1$

For the inductive step we again fixed $N \in \mathbb{N}_0$ and assume that (D.24) holds for one particular $n_0 \in \mathbb{N}$ and demonstrate that it then also holds for $n_0 + 1$. We find

$$\begin{aligned} &I_{N+2(n_0+1)}^{\pm}(\alpha,\rho) = \\ &\overset{\text{(D.22c)}}{=} f_{N+2(n_0+1)}(\alpha) I_{N+2(n_0+1)-2}^{\pm}(\alpha,\rho) + g_{N+2(n_0+1)}(\alpha,\rho) \\ &\overset{\text{(D.24)}}{=} f_{N+2(n_0+1)}(\alpha) \Big[F_{N,n_0}(\alpha) I_N^{\pm}(\alpha,\rho) + G_{N,n_0}(\alpha,\rho) \Big] + g_{N+2(n_0+1)}(\alpha,\rho) \\ &\overset{\text{(D.22a)}}{\underset{\text{(D.22b)}}{=}} f_{N+2(n_0+1)}(\alpha) \left(\prod_{i=1}^{n_0} f_{N+2i}(\alpha) \right) I_N^{\pm}(\alpha,\rho) \\ &\quad + f_{N+2(n_0+1)}(\alpha) \left[\sum_{i=0}^{n_0-1} \left(\prod_{j=0}^{i-1} f_{N+2(n_0-j)}(\alpha) \right) g_{N+2(n_0-i)}(\alpha,\rho) \right] + g_{N+2(n_0+1)} \end{aligned}$$

Absorbing the factors $f_{N+2(n_0+1)}(\alpha)$ in the first and second term into the products and rewriting the last term as $g_{N+2(n_0+1)}(\alpha,\rho) = \sum_{i=-1}^{-1} \Pi_{s=0}^{i} f_{N+2(n_0-(s-1))}(\alpha) g_{N+2(n_0-i)}(\alpha,\rho)$ we find

$$\cdots = \left(\prod_{i=1}^{n_0+1} f_{N+2i}(\alpha)\right) I_N^{\pm}(\alpha,\rho) + \left[\sum_{i=0}^{n_0-1}\left(\prod_{j=-1}^{i-1} f_{N+2(n_0-j)}(\alpha)\right) g_{N+2(n_0-i)}(\alpha,\rho)\right]$$
$$+ \sum_{i=-1}^{-1}\left(\prod_{s=0}^{i} f_{N+2(n_0-(s-1))}(\alpha)\right) g_{N+2(n_0-i)}(\alpha,\rho)$$

Performing an index shift in the product contained in the second term of the first line by setting $s = j+1$ we obtain

$$\cdots = \left(\prod_{i=1}^{n_0+1} f_{N+2i}(\alpha)\right) I_N^{\pm}(\alpha,\rho) + \left[\sum_{i=0}^{n_0-1}\left(\prod_{s=0}^{i} f_{N+2(n_0-(s-1))}(\alpha)\right) g_{N+2(n_0-i)}(\alpha,\rho)\right]$$
$$+ \sum_{i=-1}^{-1}\left(\prod_{s=0}^{i} f_{N+2(n_0-(s-1))}(\alpha)\right) g_{N+2(n_0-i)}(\alpha,\rho)$$

Combining the second term of the first line with the term in the second line and subsequently performing another index shift by setting $r = i+1$ we arrive at

$$\begin{aligned}
\cdots &= \left(\prod_{i=1}^{n_0+1} f_{N+2i}(\alpha)\right) I_N^{\pm}(\alpha,\rho) + \sum_{i=-1}^{n_0-1}\left(\prod_{s=0}^{i} f_{N+2(n_0-(s-1))}(\alpha)\right) g_{N+2(n_0-i)}(\alpha,\rho)\\
&= \left(\prod_{i=1}^{n_0+1} f_{N+2i}(\alpha)\right) I_N^{\pm}(\alpha,\rho) + \sum_{r=0}^{n_0}\left(\prod_{s=0}^{r-1} f_{N+2(n_0-(s-1))}(\alpha)\right) g_{N+2(n_0-(r-1))}(\alpha,\rho)\\
&= \left(\prod_{i=1}^{n_0+1} f_{N+2i}(\alpha)\right) I_N^{\pm}(\alpha,\rho) + \sum_{r=0}^{(n_0+1)-1}\left(\prod_{s=0}^{r-1} f_{N+2((n_0+1)-s)}(\alpha)\right) g_{N+2((n_0+1)-r)}(\alpha,\rho)\\
&\overset{\text{(D.22a)}}{\underset{\text{(D.22b)}}{=}} F_{N,n_0+1}(\alpha) I_N^{\pm}(\alpha,\rho) + G_{N,n_0+1}(\alpha,\rho)
\end{aligned} \tag{D.26}$$

which demonstrates that indeed

$$I_{N+2\tilde{n}}^{\pm}(\alpha,\rho) = F_{N,\tilde{n}}(\alpha) I_N^{\pm}(\alpha,\rho) + G_{N,\tilde{n}}(\alpha,\rho) \tag{D.27}$$

holds for all $\tilde{n} \geq 1$.

(c) Conclusion

Now, the claimed closed-form expression for $I_n^{\pm}$ with even $n \geq 4$ and odd $n \geq 5$ follow from the above result by replacing $\tilde{n} \to \frac{n-N}{2}$ and setting $N = 2$ and $N = 3$, respectively.

(2) Closed-Form Expression for $n \geq 1$

To prove the claimed relation, we demonstrate via a proof by induction on n that

$$I_{N-2n}^{\pm}(\alpha,\rho) = K_{N,n}(\alpha) I_N^{\pm}(\alpha,\rho) + L_{N,n}(\alpha,\rho) \tag{D.28}$$

holds for all $n \geq 1$ where $N \in (-\mathbb{N}_0) \cup \{0,1,2\}$ is an arbitrary, but fixed integer.

(a) Base Case $n = 1$

In the initial case, namely for $n = 1$, the claimed relations reduces to

$$I_{N-2}^{\pm}(\alpha,\rho) = K_{N,1}(\alpha) I_N^{\pm}(\alpha,\rho) + L_{N,1}(\alpha,\rho)$$

$$
\begin{aligned}
&\overset{\text{(D.23b)}}{\underset{\text{(D.23a)}}{=}} \left(\prod_{i=1}^{1} k_{N-2i}(\alpha)\right) I_N^{\pm}(\alpha,\rho) + \sum_{i=0}^{1-1}\left(\prod_{j=0}^{i-1} k_{N-2(1-j)}(\alpha)\right) l_{N-2(1-i)}(\alpha,\rho)\\
&= k_{N-2}(\alpha) I_N^{\pm}(\alpha,\rho) + \left(\prod_{j=0}^{0-1} k_{N-2(1-j)}(\alpha)\right) l_{N-2}(\alpha,\rho)\\
&= k_{N-2}(\alpha) I_N^{\pm}(\alpha,\rho) + l_{N-2}(\alpha,\rho) \qquad \text{(D.29)}
\end{aligned}
$$

which precisely is the given recursion relation (D.10) for n replaced by $N-2$. As we assumed $N \in (-\mathbb{N}_0) \cup \{0,1,2\}$ this demonstrates that the claimed relation holds for $n = 1$.

(b) Inductive Step $n_0 \to n_0 + 1$

For the inductive step we again fixed $N \in (-\mathbb{N}_0) \cup \{0,1,2\}$ and assume that (D.28) holds for one particular $n_0 \in \mathbb{N}$ and demonstrate that it then also holds for $n_0 + 1$. We find

$$
\begin{aligned}
&I^{\pm}_{N-2(n_0+1)}(\alpha,\rho) =\\
&\overset{\text{(D.22c)}}{=} k_{N-2(n_0+1)}(\alpha) I^{\pm}_{N-2(n_0+1)+2}(\alpha,\rho) + l_{N-2(n_0+1)}(\alpha,\rho)\\
&\overset{\text{(D.28)}}{=} k_{N-2(n_0+1)}(\alpha)\Big[F_{N,n_0}(\alpha) I_N^{\pm}(\alpha,\rho) + G_{N,n_0}(\alpha,\rho)\Big] + l_{N-2(n_0+1)}(\alpha,\rho)\\
&\overset{\text{(D.23a)}}{\underset{\text{(D.23b)}}{=}} k_{N-2(n_0+1)}(\alpha)\left(\prod_{i=1}^{n_0} k_{N-2i}(\alpha)\right) I_N^{\pm}(\alpha,\rho)\\
&\quad + k_{N-2(n_0+1)}(\alpha)\left[\sum_{i=0}^{n_0-1}\left(\prod_{j=0}^{i-1} k_{N-2(n_0-j)}(\alpha)\right) l_{N-2(n_0-i)}(\alpha,\rho)\right] + l_{N-2(n_0+1)}
\end{aligned}
$$

Absorbing the factors $k_{N-2(n_0+1)}(\alpha)$ in the first and second term into the products and rewriting the last term as $l_{N-2(n_0+1)}(\alpha,\rho) = \sum_{i=-1}^{-1} \Pi_{s=0}^{i} k_{N-2(n_0-(s-1))}(\alpha) l_{N-2(n_0-i)}(\alpha,\rho)$ we find

$$
\begin{aligned}
\cdots &= \left(\prod_{i=1}^{n_0+1} k_{N-2i}(\alpha)\right) I_N^{\pm}(\alpha,\rho) + \left[\sum_{i=0}^{n_0-1}\left(\prod_{j=-1}^{i-1} k_{N-2(n_0-j)}(\alpha)\right) l_{N-2(n_0-i)}(\alpha,\rho)\right]\\
&\quad + \sum_{i=-1}^{-1}\left(\prod_{s=0}^{i} k_{N-2(n_0-(s-1))}(\alpha)\right) l_{N-2(n_0-i)}(\alpha,\rho)
\end{aligned}
$$

Performing an index shift in the product contained in the second term of the first line by setting $s = j + 1$ we obtain

$$
\begin{aligned}
\cdots &= \left(\prod_{i=1}^{n_0+1} k_{N-2i}(\alpha)\right) I_N^{\pm}(\alpha,\rho) + \left[\sum_{i=0}^{n_0-1}\left(\prod_{s=0}^{i} k_{N-2(n_0-(s-1))}(\alpha)\right) l_{N-2(n_0-i)}(\alpha,\rho)\right]\\
&\quad + \sum_{i=-1}^{-1}\left(\prod_{s=0}^{i} k_{N-2(n_0-(s-1))}(\alpha)\right) l_{N-2(n_0-i)}(\alpha,\rho)
\end{aligned}
$$

Combining the second term of the first line with the term in the second line and subsequently performing another index shift by setting $r = i + 1$ we arrive at

$$
\begin{aligned}
\cdots &= \left(\prod_{i=1}^{n_0+1} k_{N-2i}(\alpha)\right) I_N^{\pm}(\alpha,\rho) + \sum_{i=-1}^{n_0-1}\left(\prod_{s=0}^{i} k_{N-2(n_0-(s-1))}(\alpha)\right) l_{N-2(n_0-i)}(\alpha,\rho)\\
&= \left(\prod_{i=1}^{n_0+1} k_{N-2i}(\alpha)\right) I_N^{\pm}(\alpha,\rho) + \sum_{r=0}^{n_0}\left(\prod_{s=0}^{r-1} k_{N-2(n_0-(s-1))}(\alpha)\right) l_{N-2(n_0-(r-1))}(\alpha,\rho)
\end{aligned}
$$

$$= \left(\prod_{i=1}^{n_0+1} k_{N-2i}(\alpha)\right) I_N^{\pm}(\alpha,\rho) + \sum_{r=0}^{(n_0+1)-1} \left(\prod_{s=0}^{r-1} k_{N-2((n_0+1)-s)}(\alpha)\right) l_{N-2((n_0+1)-r)}(\alpha,\rho)$$
$$\overset{\text{(D.23b)}}{\underset{\text{(D.23a)}}{=}} K_{N,n_0+1}(\alpha) I_N^{\pm}(\alpha,\rho) + L_{N,n_0+1}(\alpha,\rho) \tag{D.30}$$

which demonstrates that indeed

$$I_{N-2\tilde{n}}^{\pm}(\alpha,\rho) = K_{N,\tilde{n}}(\alpha) I_N^{\pm}(\alpha,\rho) + L_{N,\tilde{n}}(\alpha,\rho) \tag{D.31}$$

holds for all $\tilde{n} \geq 1$.

(c) Conclusion

Now, the claimed closed-form expression for $I_n^{\pm}$ with odd $n \leq -1$ and even $n \leq -2$ follow from the above result by replacing $\tilde{n} \to -\frac{n-N}{2}$ and setting $N = 1$ and $N = 0$, respectively.

This concludes the proof. □

We can now put together all the results to arrive at the following lemma which provides a closed-form expression for the functions $I_n^{\pm}$ for any $n \in \mathbb{Z}$.

Lemma D.2.3 (Closed-Form Expression for Functions $I_n^{\pm}$ for $n \in \mathbb{Z}$)

For $n \in \mathbb{Z}$ the functions $I_n^{\pm} : \mathbb{R}_0^+ \times (-1,1) \to \mathbb{R}$ introduced in Definition D.1.1 evaluate to

$$I_n^{\pm}(\alpha,\rho) = \begin{cases} K_{0,-\frac{n}{2}}(\alpha) I_0^{\pm}(\alpha,\rho) + L_{0,-\frac{n}{2}}(\alpha,\rho) & n \leq -2 \wedge n \text{ even} \\ K_{1,\frac{1-n}{2}}(\alpha) I_1^{\pm}(\alpha,\rho) + L_{1,\frac{1-n}{2}}(\alpha,\rho) & n \leq -1 \wedge n \text{ odd} \\ \frac{2}{\rho}\frac{s_0(\alpha,\rho)}{\alpha^2} - \frac{2}{\rho}\frac{c_{-1}(\alpha,\rho)}{\alpha} & \text{for } n = 0 \\ -\frac{2}{\rho}\frac{c_0(\alpha,\rho)}{\alpha} & \text{for } n = 1 \\ \frac{2}{\rho}\left[\mathrm{Si}(\alpha\sqrt{1+\rho}) - \mathrm{Si}(\alpha\sqrt{1-\rho})\right] & \text{for } n = 2 \\ \frac{2}{\rho}\alpha\left[\mathrm{Ci}(\alpha\sqrt{1+\rho}) - \mathrm{Ci}(\alpha\sqrt{1-\rho})\right] - \frac{2}{\rho}s_1(\alpha,\rho) & \text{for } n = 3 \\ F_{2,\frac{n-2}{2}}(\alpha) I_2^{\pm}(\alpha,\rho) + G_{2,\frac{n-2}{2}}(\alpha,\rho) & \text{for } n \geq 4 \wedge n \text{ even} \\ F_{3,\frac{n-3}{2}}(\alpha) I_3^{\pm}(\alpha,\rho) + G_{3,\frac{n-3}{2}}(\alpha,\rho) & \text{for } n \geq 5 \wedge n \text{ odd} \end{cases} \tag{D.32}$$

where the functions $F_{N,n}, G_{N,n}, K_{N,n}, L_{N,n}$ are those introduced in (D.22a), (D.22b), (D.23a) and (D.23b), respectively.

Proof. To arrive at the claimed expression, we combine the explicit expressions for $I_n^{\pm}$ where $n \in \{0,1,2,3\}$ from Proposition D.1.3 with the closed-form expressions derived in Proposition D.2.2 which together cover all cases $n \in \mathbb{Z}$. □

E

Explicit Form of Multipole Matrices at Multipole Orders $l = 0$ and $l = 1$

Contents

In this short appendix we give explicit expressions for the multipole matrices $\mathfrak{K}_0$, $\mathfrak{M}_{ll}$, $\mathfrak{N}_{ll}$ and their asterisked counterparts $\overset{*}{\mathfrak{M}}_{ll}$, $\overset{*}{\mathfrak{N}}_{ll}$ at the lowest multipole orders $l = 0$ and $l = 1$ which are obtained by evaluating Definition 4.2.11 along with the explicit expression for the eigenvalues $t_n^{\pm}$ derived in Lemma 4.2.13. For better readability and to reduce the size of the matrices, we have chosen a block representation which ultimately traces back to Definition 4.1.6 and Terminology 4.1.7.

E.1 Multipole Matrices for $l = 0$

E.1.1 Factorized Form of Trigonometric Functions

Auxiliary Calculation E.1.1 (Multipole Matrices for $l = 0$ in Factorized Form)

At multipole order $l = 0$ the multipole matrices introduced in Definition 4.2.11 read

$$\frac{\mathfrak{K}_0}{16\pi^2} = \left(\begin{array}{c|cc|c} 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times 3}} & 0 \\ \hline \mathbf{0}_{3\times 1} & \begin{array}{c} \frac{\mathrm{i}}{|\vec{p}|} \\ \mathbf{0}_{2\times 1} \end{array} & \begin{array}{c} \mathbf{0}_{1\times 2} \\ \mathbf{0}_{2\times 2} \end{array} & \mathbf{0}_{3\times 1} \\ \hline 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times 3}} & 0 \end{array}\right) \cos(|\vec{p}|r) + \left(\begin{array}{c|cc|c} 1 & \multicolumn{2}{c|}{\mathbf{0}_{1\times 3}} & 0 \\ \hline \mathbf{0}_{3\times 1} & \begin{array}{c} -\frac{\mathrm{i}}{|\vec{p}|} \\ \mathbf{0}_{2\times 1} \end{array} & \begin{array}{c} \mathbf{0}_{1\times 2} \\ \mathbf{0}_{2\times 2} \end{array} & \mathbf{0}_{3\times 1} \\ \hline 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times 3}} & 1 \end{array}\right) \frac{\sin(|\vec{p}|r)}{|\vec{p}|r} \tag{E.1a}$$

$$
\begin{aligned}
\frac{\mathfrak{M}_{00}}{16\pi^2} &= \left(\begin{array}{c|cc|c} 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \\ \hline \mathbf{0}_{3\times1} & -\frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & \mathbf{0}_{3\times1} \\ & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \\ \hline 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \end{array}\right) \cos(|\vec{p}|r)\cos(|\vec{q}|r) + \left(\begin{array}{c|cc|c} 1 & -\frac{\mathrm{i}}{|\vec{q}|} & \mathbf{0}_{1\times2} & 1 \\ \hline -\frac{\mathrm{i}}{|\vec{p}|} & -\frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & -\frac{\mathrm{i}}{|\vec{p}|} \\ \mathbf{0}_{2\times1} & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \mathbf{0}_{2\times1} \\ \hline 1 & -\frac{\mathrm{i}}{|\vec{q}|} & \mathbf{0}_{1\times2} & 1 \end{array}\right) \frac{\sin(|\vec{p}|r)}{|\vec{p}|r}\frac{\sin(|\vec{q}|r)}{|\vec{q}|r} \\
&+ \left(\begin{array}{c|cc|c} 0 & \frac{\mathrm{i}}{|\vec{q}|} & \mathbf{0}_{1\times2} & 0 \\ \hline \mathbf{0}_{3\times1} & \frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & \mathbf{0}_{3\times1} \\ & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \\ \hline 0 & \frac{\mathrm{i}}{|\vec{q}|} & \mathbf{0}_{1\times2} & 0 \end{array}\right) \frac{\sin(|\vec{p}|r)}{|\vec{p}|r}\cos(|\vec{q}|r) + \left(\begin{array}{c|cc|c} 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \\ \hline \frac{\mathrm{i}}{|\vec{p}|} & \frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & \frac{\mathrm{i}}{|\vec{p}|} \\ \mathbf{0}_{2\times1} & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \mathbf{0}_{2\times1} \\ \hline 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \end{array}\right) \cos(|\vec{p}|r)\frac{\sin(|\vec{q}|r)}{|\vec{q}|r}
\end{aligned} \tag{E.1b}
$$

$$
\begin{aligned}
\frac{\mathfrak{N}_{00}}{16\pi^2} &= \left(\begin{array}{c|cc|c} 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \\ \hline \mathbf{0}_{3\times1} & \frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & \mathbf{0}_{3\times1} \\ & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \\ \hline 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \end{array}\right) \cos(|\vec{p}|r)\cos(|\vec{q}|r) + \left(\begin{array}{c|cc|c} 1 & \frac{\mathrm{i}}{|\vec{q}|} & \mathbf{0}_{1\times2} & 1 \\ \hline -\frac{\mathrm{i}}{|\vec{p}|} & \frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & -\frac{\mathrm{i}}{|\vec{p}|} \\ \mathbf{0}_{2\times1} & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \mathbf{0}_{2\times1} \\ \hline 1 & \frac{\mathrm{i}}{|\vec{q}|} & \mathbf{0}_{1\times2} & 1 \end{array}\right) \frac{\sin(|\vec{p}|r)}{|\vec{p}|r}\frac{\sin(|\vec{q}|r)}{|\vec{q}|r} \\
&+ \left(\begin{array}{c|cc|c} 0 & -\frac{\mathrm{i}}{|\vec{q}|} & \mathbf{0}_{1\times2} & 0 \\ \hline \mathbf{0}_{3\times1} & -\frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & \mathbf{0}_{3\times1} \\ & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \\ \hline 0 & -\frac{\mathrm{i}}{|\vec{q}|} & \mathbf{0}_{1\times2} & 0 \end{array}\right) \frac{\sin(|\vec{p}|r)}{|\vec{p}|r}\cos(|\vec{q}|r) + \left(\begin{array}{c|cc|c} 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \\ \hline \frac{\mathrm{i}}{|\vec{p}|} & -\frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & \frac{\mathrm{i}}{|\vec{p}|} \\ \mathbf{0}_{2\times1} & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \mathbf{0}_{2\times1} \\ \hline 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \end{array}\right) \cos(|\vec{p}|r)\frac{\sin(|\vec{q}|r)}{|\vec{q}|r}
\end{aligned} \tag{E.1c}
$$

$$
\begin{aligned}
\frac{\overset{*}{\mathfrak{M}}_{00}}{16\pi^2} &= \left(\begin{array}{c|cc|c} 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \\ \hline \mathbf{0}_{3\times1} & -\frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & \mathbf{0}_{3\times1} \\ & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \\ \hline 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \end{array}\right) \frac{\cos(|\vec{p}|r)}{|\vec{p}|r}\frac{\cos(|\vec{q}|r)}{|\vec{q}|r} + \left(\begin{array}{c|cc|c} 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \\ \hline \mathbf{0}_{3\times1} & -\frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & \mathbf{0}_{3\times1} \\ & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \\ \hline 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \end{array}\right) \frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^2}\frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^2} \\
&+ \left(\begin{array}{c|cc|c} 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \\ \hline \mathbf{0}_{3\times1} & \frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & \mathbf{0}_{3\times1} \\ & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \\ \hline 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \end{array}\right) \frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^2}\frac{\cos(|\vec{q}|r)}{|\vec{q}|r} + \left(\begin{array}{c|cc|c} 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \\ \hline \mathbf{0}_{3\times1} & \frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & \mathbf{0}_{3\times1} \\ & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \\ \hline 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \end{array}\right) \frac{\cos(|\vec{p}|r)}{|\vec{p}|r}\frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^2}
\end{aligned} \tag{E.1d}
$$

$$
\begin{aligned}
\frac{\overset{*}{\mathfrak{N}}_{00}}{16\pi^2} &= \left(\begin{array}{c|cc|c} 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \\ \hline \mathbf{0}_{3\times1} & \frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & \mathbf{0}_{3\times1} \\ & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \\ \hline 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \end{array}\right) \frac{\cos(|\vec{p}|r)}{|\vec{p}|r}\frac{\cos(|\vec{q}|r)}{|\vec{q}|r} + \left(\begin{array}{c|cc|c} 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \\ \hline \mathbf{0}_{3\times1} & \frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & \mathbf{0}_{3\times1} \\ & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \\ \hline 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \end{array}\right) \frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^2}\frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^2} \\
&+ \left(\begin{array}{c|cc|c} 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \\ \hline \mathbf{0}_{3\times1} & -\frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & \mathbf{0}_{3\times1} \\ & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \\ \hline 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \end{array}\right) \frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^2}\frac{\cos(|\vec{q}|r)}{|\vec{q}|r} + \left(\begin{array}{c|cc|c} 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \\ \hline \mathbf{0}_{3\times1} & -\frac{1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times2} & \mathbf{0}_{3\times1} \\ & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \\ \hline 0 & \multicolumn{2}{c|}{\mathbf{0}_{1\times3}} & 0 \end{array}\right) \frac{\cos(|\vec{p}|r)}{|\vec{p}|r}\frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^2}
\end{aligned} \tag{E.1e}
$$

Proof. To arrive at the claimed expressions we insert the explicit form of the eigenvalues $t_n^{\pm}$ as derived in Lemma 4.2.13 into Definition 4.2.11, evaluate at $l = 0$ and factorize the trigonometric functions. □

E.1.2 Non-Factorized Form of Trigonometric Functions

The calculations in Subsection 6.1.3 simplify considerably if the matrices are given with trigonometric functions having arguments $|\vec{p}| \pm |\vec{q}|$.

Auxiliary Calculation E.1.2 (Multipole Matrix $\mathfrak{N}_{00}$ in Non-Factorized Form)

At multipole order $l = 0$ the multipole matrix $\mathfrak{N}_{00}$ in non-factorized form reads

$$
\begin{aligned}
\frac{\mathfrak{N}_{00}}{8\pi^2} = {}& \left(\begin{array}{c|cc|c}
-1 & -\frac{\mathrm{i}}{|\vec{q}|} & \mathbf{0}_{1\times 2} & -1 \\ \hline
\frac{\mathrm{i}}{|\vec{p}|} & \frac{(|\vec{p}|r)(|\vec{q}|r)-1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times 2} & \frac{\mathrm{i}}{|\vec{p}|} \\
\mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 1} \\ \hline
-1 & -\frac{\mathrm{i}}{|\vec{q}|} & \mathbf{0}_{1\times 2} & -1
\end{array}\right) \frac{\cos\left[(|\vec{p}|+|\vec{q}|)r\right]}{(|\vec{p}|r)(|\vec{q}|r)}
+ \left(\begin{array}{c|cc|c}
1 & \frac{\mathrm{i}}{|\vec{q}|} & \mathbf{0}_{1\times 2} & 1 \\ \hline
-\frac{\mathrm{i}}{|\vec{p}|} & \frac{(|\vec{p}|r)(|\vec{q}|r)+1}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times 2} & -\frac{\mathrm{i}}{|\vec{p}|} \\
\mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 1} \\ \hline
1 & \frac{\mathrm{i}}{|\vec{q}|} & \mathbf{0}_{1\times 2} & 1
\end{array}\right) \frac{\cos\left[(|\vec{p}|-|\vec{q}|)r\right]}{(|\vec{p}|r)(|\vec{q}|r)} \\
&+ \left(\begin{array}{c|cc|c}
0 & -\mathrm{i}r & \mathbf{0}_{1\times 2} & 0 \\ \hline
\mathrm{i}r & -\frac{(|\vec{p}|+|\vec{q}|)r}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times 2} & \mathrm{i}r \\
\mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 1} \\ \hline
0 & -\mathrm{i}r & \mathbf{0}_{1\times 2} & 0
\end{array}\right) \frac{\sin\left[(|\vec{p}|+|\vec{q}|)r\right]}{(|\vec{p}|r)(|\vec{q}|r)}
+ \left(\begin{array}{c|cc|c}
0 & -\mathrm{i}r & \mathbf{0}_{1\times 2} & 0 \\ \hline
-\mathrm{i}r & \frac{(|\vec{p}|-|\vec{q}|)r}{|\vec{p}||\vec{q}|} & \mathbf{0}_{1\times 2} & -\mathrm{i}r \\
\mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 1} \\ \hline
0 & -\mathrm{i}r & \mathbf{0}_{1\times 2} & 0
\end{array}\right) \frac{\sin\left[(|\vec{p}|-|\vec{q}|)r\right]}{(|\vec{p}|r)(|\vec{q}|r)}
\end{aligned}
\tag{E.2a}
$$

Proof. To arrive at the claimed expressions we insert the explicit form of the eigenvalues $t_n^{\pm}$ as derived in Lemma 4.2.13 into Definition 4.2.11, evaluate at $l = 0$ and factorize the trigonometric functions. □

E.2 Multipole Matrices at Multipole Order $l = 1$

For the evaluation of the second variation of the iε-regularized causal action for Lorentz boosts in Appendix F it is most convenient to have the multipole matrices for $l = 1$ with the trigonometric functions in factorized form.

Auxiliary Calculation E.2.1 (Multipole Matrices for $l = 1$ in Factorized Form)

At multipole order $l = 1$ the multipole matrices introduced in Definition 4.2.11 read

$$
\begin{aligned}
\frac{\mathfrak{M}_{11}}{16\pi^2} = {}& \left(\begin{array}{c|ccc|c}
-1 & \frac{2\mathrm{i}}{|\vec{q}|} & -\frac{2\mathrm{i}}{|\vec{q}|} & 0 & -1 \\ \hline
\frac{2\mathrm{i}}{|\vec{p}|} & \frac{4}{|\vec{p}||\vec{q}|} & -\frac{4}{|\vec{p}||\vec{q}|} & 0 & \frac{2\mathrm{i}}{|\vec{p}|} \\
-\frac{2\mathrm{i}}{|\vec{p}|} & -\frac{4}{|\vec{p}||\vec{q}|} & -\frac{4}{|\vec{p}||\vec{q}|} & 0 & -\frac{2\mathrm{i}}{|\vec{p}|} \\
0 & 0 & 0 & 0 & 0 \\ \hline
-1 & \frac{2\mathrm{i}}{|\vec{q}|} & -\frac{2\mathrm{i}}{|\vec{q}|} & 0 & -1
\end{array}\right) \frac{\cos(|\vec{p}|r)}{|\vec{p}|r}\,\frac{\cos(|\vec{q}|r)}{|\vec{q}|r} \\
&+ \left(\begin{array}{c|ccc|c}
-1 & -\frac{\mathrm{i}[(|\vec{q}|r)^2-2]}{|\vec{q}|} & -\frac{2\mathrm{i}}{|\vec{q}|} & 0 & -1 \\ \hline
-\frac{\mathrm{i}[(|\vec{p}|r)^2-2]}{|\vec{p}|} & \frac{[(|\vec{p}|r)^2-2][(|\vec{q}|r)^2-2]}{|\vec{p}||\vec{q}|} & \frac{2[(|\vec{p}|r)^2-2]}{|\vec{p}||\vec{q}|} & 0 & -\frac{\mathrm{i}[(|\vec{p}|r)^2-2]}{|\vec{p}|} \\
-\frac{2\mathrm{i}}{|\vec{p}|} & \frac{2[(|\vec{q}|r)^2-2]}{|\vec{p}||\vec{q}|} & -\frac{4}{|\vec{p}||\vec{q}|} & 0 & -\frac{2\mathrm{i}}{|\vec{p}|} \\
0 & 0 & 0 & 0 & 0 \\ \hline
-1 & -\frac{\mathrm{i}[(|\vec{q}|r)^2-2]}{|\vec{q}|} & -\frac{2\mathrm{i}}{|\vec{q}|} & 0 & -1
\end{array}\right) \frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^2}\,\frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^2} \\
&+ \left(\begin{array}{c|ccc|c}
1 & -\frac{2\mathrm{i}}{|\vec{q}|} & \frac{2\mathrm{i}}{|\vec{q}|} & 0 & 1 \\ \hline
\frac{\mathrm{i}[(|\vec{p}|r)^2-2]}{|\vec{p}|} & \frac{2[(|\vec{p}|r)^2-2]}{|\vec{p}||\vec{q}|} & -\frac{2[(|\vec{p}|r)^2-2]}{|\vec{p}||\vec{q}|} & 0 & \frac{\mathrm{i}[(|\vec{p}|r)^2-2]}{|\vec{p}|} \\
\frac{2\mathrm{i}}{|\vec{p}|} & \frac{4}{|\vec{p}||\vec{q}|} & \frac{4}{|\vec{p}||\vec{q}|} & 0 & \frac{2\mathrm{i}}{|\vec{p}|} \\
0 & 0 & 0 & 0 & 0 \\ \hline
1 & -\frac{2\mathrm{i}}{|\vec{q}|} & \frac{2\mathrm{i}}{|\vec{q}|} & 0 & 1
\end{array}\right) \frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^2}\,\frac{\cos(|\vec{q}|r)}{|\vec{q}|r} \\
&+ \left(\begin{array}{c|ccc|c}
1 & \frac{\mathrm{i}[(|\vec{q}|r)^2-2]}{|\vec{q}|} & \frac{2\mathrm{i}}{|\vec{q}|} & 0 & 1 \\ \hline
-\frac{2\mathrm{i}}{|\vec{p}|} & \frac{2[(|\vec{q}|r)^2-2]}{|\vec{p}||\vec{q}|} & \frac{4}{|\vec{p}||\vec{q}|} & 0 & -\frac{2\mathrm{i}}{|\vec{p}|} \\
\frac{2\mathrm{i}}{|\vec{p}|} & -\frac{2[(|\vec{q}|r)^2-2]}{|\vec{p}||\vec{q}|} & \frac{4}{|\vec{p}||\vec{q}|} & 0 & \frac{2\mathrm{i}}{|\vec{p}|} \\
0 & 0 & 0 & 0 & 0 \\ \hline
1 & \frac{\mathrm{i}[(|\vec{q}|r)^2-2]}{|\vec{q}|} & \frac{2\mathrm{i}}{|\vec{q}|} & 0 & 1
\end{array}\right) \frac{\cos(|\vec{p}|r)}{|\vec{p}|r}\,\frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^2}
\end{aligned}
\tag{E.3a}
$$

$$
\begin{aligned}
\frac{\mathfrak{N}_{11}}{16\pi^2} = {} & \left(\begin{array}{c|ccc|c}
1 & \frac{2\mathrm{i}}{|\vec{q}|} & -\frac{2\mathrm{i}}{|\vec{q}|} & 0 & 1 \\
\hline
-\frac{2\mathrm{i}}{|\vec{p}|} & \frac{4}{|\vec{p}||\vec{q}|} & -\frac{4}{|\vec{p}||\vec{q}|} & 0 & -\frac{2\mathrm{i}}{|\vec{p}|} \\
\frac{2\mathrm{i}}{|\vec{p}|} & -\frac{4}{|\vec{p}||\vec{q}|} & -\frac{4}{|\vec{p}||\vec{q}|} & 0 & \frac{2\mathrm{i}}{|\vec{p}|} \\
0 & 0 & 0 & 0 & 0 \\
\hline
1 & \frac{2\mathrm{i}}{|\vec{q}|} & -\frac{2\mathrm{i}}{|\vec{q}|} & 0 & 1
\end{array}\right) \frac{\cos(|\vec{p}|r)}{|\vec{p}|r} \frac{\cos(|\vec{q}|r)}{|\vec{q}|r} \\
& + \left(\begin{array}{c|ccc|c}
1 & -\frac{\mathrm{i}[(|\vec{q}|r)^2-2]}{|\vec{q}|} & -\frac{2\mathrm{i}}{|\vec{q}|} & 0 & 1 \\
\hline
\frac{\mathrm{i}[(|\vec{p}|r)^2-2]}{|\vec{p}|} & \frac{[(|\vec{p}|r)^2-2][(|\vec{q}|r)^2-2]}{|\vec{p}||\vec{q}|} & \frac{2[(|\vec{p}|r)^2-2]}{|\vec{p}||\vec{q}|} & 0 & \frac{\mathrm{i}[(|\vec{p}|r)^2-2]}{|\vec{p}|} \\
\frac{2\mathrm{i}}{|\vec{p}|} & \frac{2[(|\vec{q}|r)^2-2]}{|\vec{p}||\vec{q}|} & -\frac{4}{|\vec{p}||\vec{q}|} & 0 & \frac{2\mathrm{i}}{|\vec{p}|} \\
0 & 0 & 0 & 0 & 0 \\
\hline
1 & -\frac{\mathrm{i}[(|\vec{q}|r)^2-2]}{|\vec{q}|} & -\frac{2\mathrm{i}}{|\vec{q}|} & 0 & 1
\end{array}\right) \frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^2} \frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^2} \\
& + \left(\begin{array}{c|ccc|c}
-1 & -\frac{2\mathrm{i}}{|\vec{q}|} & \frac{2\mathrm{i}}{|\vec{q}|} & 0 & -1 \\
\hline
-\frac{\mathrm{i}[(|\vec{p}|r)^2-2]}{|\vec{p}|} & \frac{2[(|\vec{p}|r)^2-2]}{|\vec{p}||\vec{q}|} & -\frac{2[(|\vec{p}|r)^2-2]}{|\vec{p}||\vec{q}|} & 0 & -\frac{\mathrm{i}[(|\vec{p}|r)^2-2]}{|\vec{p}|} \\
-\frac{2\mathrm{i}}{|\vec{p}|} & \frac{4}{|\vec{p}||\vec{q}|} & \frac{4}{|\vec{p}||\vec{q}|} & 0 & -\frac{2\mathrm{i}}{|\vec{p}|} \\
0 & 0 & 0 & 0 & 0 \\
\hline
-1 & -\frac{2\mathrm{i}}{|\vec{q}|} & \frac{2\mathrm{i}}{|\vec{q}|} & 0 & -1
\end{array}\right) \frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^2} \frac{\cos(|\vec{q}|r)}{|\vec{q}|r} \\
& + \left(\begin{array}{c|ccc|c}
-1 & \frac{\mathrm{i}[(|\vec{q}|r)^2-2]}{|\vec{q}|} & \frac{2\mathrm{i}}{|\vec{q}|} & 0 & -1 \\
\hline
\frac{2\mathrm{i}}{|\vec{p}|} & \frac{2[(|\vec{q}|r)^2-2]}{|\vec{p}||\vec{q}|} & \frac{4}{|\vec{p}||\vec{q}|} & 0 & \frac{2\mathrm{i}}{|\vec{p}|} \\
-\frac{2\mathrm{i}}{|\vec{p}|} & -\frac{2[(|\vec{q}|r)^2-2]}{|\vec{p}||\vec{q}|} & \frac{4}{|\vec{p}||\vec{q}|} & 0 & -\frac{2\mathrm{i}}{|\vec{p}|} \\
0 & 0 & 0 & 0 & 0 \\
\hline
-1 & \frac{\mathrm{i}[(|\vec{q}|r)^2-2]}{|\vec{q}|} & \frac{2\mathrm{i}}{|\vec{q}|} & 0 & -1
\end{array}\right) \frac{\cos(|\vec{p}|r)}{|\vec{p}|r} \frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^2}
\end{aligned}
\tag{E.3b}
$$

$$
\begin{aligned}
\frac{\overset{*}{\mathfrak{M}}_{11}}{4\pi^2} = {} & \left(\begin{array}{c|ccc|c}
0 & & \mathbf{0}_{1\times 3} & & 0 \\
\hline
 & 24 & -24 & 0 & \\
\mathbf{0}_{3\times 1} & -24 & [((|\vec{p}|r)^2-(|\vec{q}|r)^2)^2+24] & 0 & \mathbf{0}_{3\times 1} \\
 & 0 & 0 & 0 & \\
\hline
0 & & \mathbf{0}_{1\times 3} & & 0
\end{array}\right) \frac{\cos(|\vec{p}|r)}{(|\vec{p}|r)^2} \frac{\cos(|\vec{q}|r)}{(|\vec{q}|r)^2} \\
& + \left(\begin{array}{c|ccc|c}
0 & & \mathbf{0}_{1\times 3} & & 0 \\
\hline
 & \begin{matrix} 4[(|\vec{p}|r)^2(|\vec{q}|r)^2 \\ -2((|\vec{p}|r)^2+(|\vec{q}|r)^2)+6] \end{matrix} & \begin{matrix} -[((|\vec{p}|r)^2-(|\vec{q}|r)^2)^2 \\ -8((|\vec{p}|r)^2+(|\vec{q}|r)^2)+24] \end{matrix} & 0 & \\
\mathbf{0}_{3\times 1} & \begin{matrix} -[((|\vec{p}|r)^2-(|\vec{q}|r)^2)^2 \\ -8((|\vec{p}|r)^2+(|\vec{q}|r)^2)+24] \end{matrix} & \begin{matrix} 4[((|\vec{p}|r)^4+(|\vec{q}|r)^4) \\ -2((|\vec{p}|r)^2+(|\vec{q}|r)^2)+6] \end{matrix} & 0 & \mathbf{0}_{3\times 1} \\
 & 0 & 0 & 0 & \\
\hline
0 & & \mathbf{0}_{1\times 3} & & 0
\end{array}\right) \frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^3} \frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^3} \\
& + \left(\begin{array}{c|ccc|c}
0 & & \mathbf{0}_{1\times 3} & & 0 \\
\hline
 & 8[(|\vec{p}|r)^2-3] & \begin{matrix} [(|\vec{p}|r)^2((|\vec{p}|r)^2-(|\vec{q}|r)^2)) \\ -8(|\vec{p}|r)^2+24] \end{matrix} & 0 & \\
\mathbf{0}_{3\times 1} & \begin{matrix} [(|\vec{p}|r)^2((|\vec{p}|r)^2-(|\vec{q}|r)^2) \\ -8(|\vec{p}|r)^2+24] \end{matrix} & \begin{matrix} -[-5(|\vec{p}|r)^2(|\vec{q}|r)^2+(|\vec{q}|r)^4 \\ +4(|\vec{p}|r)^4-8(|\vec{p}|r)^2+24] \end{matrix} & 0 & \mathbf{0}_{3\times 1} \\
 & 0 & 0 & 0 & \\
\hline
0 & & \mathbf{0}_{1\times 3} & & 0
\end{array}\right) \frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^3} \frac{\cos(|\vec{q}|r)}{(|\vec{q}|r)^2} \\
& + \left(\begin{array}{c|ccc|c}
0 & & \mathbf{0}_{1\times 3} & & 0 \\
\hline
 & 8[(|\vec{q}|r)^2-3] & \begin{matrix} [(|\vec{q}|r)^2((|\vec{q}|r)^2-(|\vec{p}|r)^2)) \\ -8(|\vec{q}|r)^2+24] \end{matrix} & 0 & \\
\mathbf{0}_{3\times 1} & \begin{matrix} [(|\vec{p}|r)^2((|\vec{q}|r)^2-(|\vec{p}|r)^2) \\ -8(|\vec{p}|r)^2+24] \end{matrix} & \begin{matrix} -[-5(|\vec{p}|r)^2(|\vec{q}|r)^2+(|\vec{p}|r)^4 \\ +4(|\vec{q}|r)^4-8(|\vec{q}|r)^2+24] \end{matrix} & 0 & \mathbf{0}_{3\times 1} \\
 & 0 & 0 & 0 & \\
\hline
0 & & \mathbf{0}_{1\times 3} & & 0
\end{array}\right) \frac{\cos(|\vec{p}|r)}{(|\vec{p}|r)^2} \frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^3}
\end{aligned}
\tag{E.3c}
$$

$$
\begin{aligned}
\frac{\overset{*}{\mathfrak{N}}_{11}}{4\pi^2} = {}& \left(\begin{array}{c|ccc|c}
0 & & \mathbf{0}_{1\times 3} & & 0 \\ \hline
 & 24 & -24 & 0 & \\
\mathbf{0}_{3\times 1} & -24 & [((|\vec{p}|r)^2 - (|\vec{q}|r)^2)^2 + 24] & 0 & \mathbf{0}_{3\times 1} \\
 & 0 & 0 & 0 & \\ \hline
0 & & \mathbf{0}_{1\times 3} & & 0
\end{array}\right) \frac{\cos(|\vec{p}|r)}{(|\vec{p}|r)^2} \frac{\cos(|\vec{q}|r)}{(|\vec{q}|r)^2} \\
& + \left(\begin{array}{c|ccc|c}
0 & & \mathbf{0}_{1\times 3} & & 0 \\ \hline
 & \begin{array}{c} 4[(|\vec{p}|r)^2(|\vec{q}|r)^2 \\ -2((|\vec{p}|r)^2+(|\vec{q}|r)^2)+6] \end{array} & \begin{array}{c} -[((|\vec{p}|r)^2-(|\vec{q}|r)^2)^2 \\ -8((|\vec{p}|r)^2+(|\vec{q}|r)^2)+24] \end{array} & 0 & \\
\mathbf{0}_{3\times 1} & \begin{array}{c} -[((|\vec{p}|r)^2-(|\vec{q}|r)^2)^2 \\ -8((|\vec{p}|r)^2+(|\vec{q}|r)^2)+24] \end{array} & \begin{array}{c} 4[((|\vec{p}|r)^4+(|\vec{q}|r)^4) \\ -2((|\vec{p}|r)^2+(|\vec{q}|r)^2)+6] \end{array} & 0 & \mathbf{0}_{3\times 1} \\
 & 0 & 0 & 0 & \\ \hline
0 & & \mathbf{0}_{1\times 3} & & 0
\end{array}\right) \frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^3} \frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^3} \\
& + \left(\begin{array}{c|ccc|c}
0 & & \mathbf{0}_{1\times 3} & & 0 \\ \hline
 & 8[(|\vec{p}|r)^2 - 3] & \begin{array}{r} [(|\vec{p}|r)^2((|\vec{p}|r)^2-(|\vec{q}|r)^2)) \\ -8(|\vec{p}|r)^2+24] \end{array} & 0 & \\
\mathbf{0}_{3\times 1} & \begin{array}{r} [(|\vec{p}|r)^2((|\vec{p}|r)^2-(|\vec{q}|r)^2) \\ -8(|\vec{p}|r)^2+24] \end{array} & \begin{array}{r} -[-5(|\vec{p}|r)^2(|\vec{q}|r)^2+(|\vec{q}|r)^4 \\ +4(|\vec{p}|r)^4-8(|\vec{p}|r)^2+24] \end{array} & 0 & \mathbf{0}_{3\times 1} \\
 & 0 & 0 & 0 & \\ \hline
0 & & \mathbf{0}_{1\times 3} & & 0
\end{array}\right) \frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^3} \frac{\cos(|\vec{q}|r)}{(|\vec{q}|r)^2} \\
& + \left(\begin{array}{c|ccc|c}
0 & & \mathbf{0}_{1\times 3} & & 0 \\ \hline
 & 8[(|\vec{q}|r)^2 - 3] & \begin{array}{r} [(|\vec{q}|r)^2((|\vec{q}|r)^2-(|\vec{p}|r)^2)) \\ -8(|\vec{q}|r)^2+24] \end{array} & 0 & \\
\mathbf{0}_{3\times 1} & \begin{array}{r} [(|\vec{p}|r)^2((|\vec{q}|r)^2-(|\vec{p}|r)^2) \\ -8(|\vec{p}|r)^2+24] \end{array} & \begin{array}{r} -[-5(|\vec{p}|r)^2(|\vec{q}|r)^2+(|\vec{p}|r)^4 \\ +4(|\vec{q}|r)^4-8(|\vec{q}|r)^2+24] \end{array} & 0 & \mathbf{0}_{3\times 1} \\
 & 0 & 0 & 0 & \\ \hline
0 & & \mathbf{0}_{1\times 3} & & 0
\end{array}\right) \frac{\cos(|\vec{p}|r)}{(|\vec{p}|r)^2} \frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^3}
\end{aligned}
\tag{E.3d}
$$

Proof. To arrive at the claimed expressions we insert the explicit form of the eigenvalues $t_n^\pm$ as derived in Lemma 4.2.13 into Definition 4.2.11, evaluate at $l = 0$ and factorize the trigonometric functions. □

F

Evaluation of $\delta^2\mathcal{S}^\varepsilon$ for Lorentz Boosts

Contents

In this appendix we evaluate the angular-integrated incomplete Fourier transforms which enter the calculation of $\delta^2\mathcal{S}^\varepsilon$ for Lorentz boosts.

F.1 Condensed Incomplete Fourier Transforms

In order to benefit from the compact notation provided by the Hadamard product, we start by rewriting the incomplete Fourier transforms from Lemma 4.2.12 as traces of Hadamard products involving the coefficient matrices and the multipole matrices.

Proposition F.1.1 (Hadamard Product Form of Lemma 4.2.12)

The non-vanishing condensed incomplete Fourier transforms as defined in Definition 5.1.3 can be expressed in terms of Hadamard products as

$$\left\{\mathcal{F}\left[\mathcal{K}^\varepsilon_{00}\right]\right\} = \int_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0, r)\ \frac{r^2 E^\varepsilon_{\mathcal{K}}}{\sqrt{4\pi}} \operatorname{tr}\left[\mathcal{C}^\varepsilon_{\mathcal{K}}\left(\mathcal{Z}_{\mathcal{K}} \odot \mathfrak{K}^{\mathrm{T}}_0\right)\right] \tag{F.1a}$$

$$\begin{Bmatrix} \left\{\mathcal{F}\left[\mathcal{M}^\varepsilon_{lm|l(-m)}\right]\right\} \\ \left\{\mathcal{F}\left[\mathcal{N}^\varepsilon_{lm|l(-m)}\right]\right\} \end{Bmatrix} = \int_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0, r) \begin{Bmatrix} (-1)^m r^2 E^\varepsilon_{\mathcal{M}} \operatorname{tr}\left[\mathcal{C}^\varepsilon_{\mathcal{M}}\left(\mathcal{Z} \odot \mathfrak{M}^{\mathrm{T}}_{ll}\right) + C^\varepsilon \mathbb{1}_5\left(\mathcal{Z} \odot \overset{*}{\mathfrak{M}}{}^{\mathrm{T}}_{ll}\right)\right] \\ r^2 E^\varepsilon_{\mathcal{N}} \operatorname{tr}\left[\mathcal{C}^\varepsilon_{\mathcal{N}}\left(\mathcal{Z} \odot \mathfrak{N}^{\mathrm{T}}_{ll}\right) - B^\varepsilon \mathbb{1}_5\left(\mathcal{Z} \odot \overset{*}{\mathfrak{N}}{}^{\mathrm{T}}_{ll}\right)\right] \end{Bmatrix} \tag{F.1b}$$

$$\begin{Bmatrix} \left\{\mathcal{F}\left[\mathcal{V}^\varepsilon_{lm|l(-m)}\right]\right\} \\ \left\{\mathcal{F}\left[\mathcal{W}^\varepsilon_{lm|l(-m)}\right]\right\} \end{Bmatrix} = \int_{\mathbb{R}} \mathrm{d}\xi^0 \left.\begin{Bmatrix} (-1)^m r^2 E^\varepsilon_{\mathcal{V}} \operatorname{tr}\left[\mathcal{C}^\varepsilon_{\mathcal{V}}\left(\mathcal{Z} \odot \mathfrak{M}^{\mathrm{T}}_{ll}\right)\right] \\ r^2 E^\varepsilon_{\mathcal{W}} \operatorname{tr}\left[\mathcal{C}^\varepsilon_{\mathcal{W}}\left(\mathcal{Z} \odot \mathfrak{N}^{\mathrm{T}}_{ll}\right)\right] \end{Bmatrix}\right|_{r=R^\varepsilon_{\max}(\xi^0)} \tag{F.1c}$$

where we suppressed the momentum arguments of the incomplete Fourier transforms. The matrices $\mathcal{Z}_{\mathcal{K}}$ and $\mathcal{Z}$ appearing in the above expressions are defined as

$$\mathcal{Z}_{\mathcal{K}} = \left(\begin{array}{c|cc|c} -\omega(|\vec{p}|) & -\omega(|\vec{p}|) & \mathbf{0}_{1\times 2} & -\omega(|\vec{p}|) \\ \hline |\vec{p}| & |\vec{p}| & \mathbf{0}_{1\times 2} & |\vec{p}| \\ \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 1} \\ \hline \mu & \mu & \mathbf{0}_{1\times 2} & \mu \end{array}\right) \tag{F.2a}$$

$$\mathcal{Z} = \left(\begin{array}{c|cc|c} \omega(|\vec{p}|)\omega(|\vec{q}|) & -|\vec{p}|\omega(|\vec{q}|) & \mathbf{0}_{1\times 2} & -\mu\omega(|\vec{q}|) \\ \hline -\,\omega(|\vec{p}|)|\vec{q}| & |\vec{p}||\vec{q}| & \mathbf{0}_{1\times 2} & \mu|\vec{q}| \\ \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 1} \\ \hline -\,\mu\omega(|\vec{p}|) & \mu|\vec{p}| & \mathbf{0}_{1\times 2} & \mu^2 \end{array}\right) \tag{F.2b}$$

Proof. To prove the statement, we make use of the following property of the Hadamard product: Let $A, B \in \mathbb{C}^{n\times n}$ and $v, w \in \mathbb{C}^n$ be given matrices and vectors, respectively, and let D_v, D_w denote the $n \times n$ diagonal matrices with entries given by

$$(D_v)_{ij} = \delta_{ij} v_i \qquad \text{and} \qquad (D_w)_{ij} = \delta_{ij} w_i$$

By making use of the definition of the Hadamard product and the matrices D_v, D_w, an inner product of the form $\overline{v}^{\mathrm{T}}(A \odot B)w$ can be rewritten as a trace in the following way

$$\begin{aligned} \overline{v}^{\mathrm{T}}(A \odot B)w &= \sum_{i,j=1}^{n} \overline{v}_i (A \odot B)_{ij} w_j = \sum_{i,j=1}^{n} \overline{v}_i A_{ij} w_j (B^{\mathrm{T}})_{ji} \\ &= \sum_{i,j=1}^{n} \sum_{k,l=1}^{n} \overline{v}_i \delta_{ik} A_{kl} \delta_{lj} w_j (B^{\mathrm{T}})_{ji} = \sum_{i=1}^{n} \left[\sum_{j,k,l=1}^{n} (D_{\overline{v}})_{ik} A_{kl} (D_w)_{lj} (B^{\mathrm{T}})_{ji} \right] \\ &= \operatorname{tr}\left(D_{\overline{v}} A D_w B^{\mathrm{T}} \right) \end{aligned}$$

In order to combine the matrices $D_{\overline{v}}$ and D_w into one object, we first exploit the cyclicity of the trace and subsequently make use the relation

$$\begin{aligned} \left(D_w B^{\mathrm{T}} D_{\overline{v}} \right)_{ij} &= \sum_{k,l=1}^{n} (D_w)_{ik} (B^{\mathrm{T}})_{kl} (D_{\overline{v}})_{lj} = \sum_{k,l=1}^{n} w_i \delta_{ik} (B^{\mathrm{T}})_{kl} \delta_{lj} \overline{v}_j \\ &= w_i (B^{\mathrm{T}})_{ij} \overline{v}_j = (w\overline{v}^{\mathrm{T}})_{ij} (B^{\mathrm{T}})_{ij} = \left((w\overline{v}^{\mathrm{T}}) \odot B^{\mathrm{T}} \right)_{ij} \end{aligned}$$

In this way, the initial inner product can be cast into the form

$$\overline{v}^{\mathrm{T}}(A \odot B)w = \operatorname{tr}\left[A\big(\mathcal{Z} \odot B^{\mathrm{T}}\big) \right] \qquad \text{where} \qquad \mathcal{Z} := w\overline{v}^{\mathrm{T}}$$

By identifying the matrices A, B and vectors v, w in the above relation as

$$A \equiv \mathcal{C}^{\varepsilon}_{\mathcal{M}}, \quad B \equiv \mathfrak{M}_{ll'} \qquad \text{and} \qquad v \equiv \begin{pmatrix} p^0 \\ |\vec{p}| \\ 0 \\ 0 \\ \mu \end{pmatrix}, \quad w \equiv \begin{pmatrix} q^0 \\ |\vec{q}| \\ 0 \\ 0 \\ \mu \end{pmatrix}$$

the condensed incomplete Fourier transform of $\mathcal{F}\big[\mathcal{M}^{\varepsilon}_{lm|l(-m)}\big]$ as given in (4.44b) takes the form

$$\Big\{ \mathcal{F}\big[\mathcal{M}^{\varepsilon}_{lm|l(-m)}\big] \Big\} = \int_{\mathcal{X}^{\varepsilon}} \mathrm{d}(\xi^0, r) \; (-1)^m r^2 E^{\varepsilon}_{\mathcal{M}} \bigg(\operatorname{tr}\Big[\mathcal{C}^{\varepsilon}_{\mathcal{M}} \big(\mathcal{Z} \odot \mathfrak{M}^{\mathrm{T}}_{ll} \big) \Big] + C^{\varepsilon} \operatorname{tr}\Big[\mathbb{1}_5 \big(\mathcal{Z} \odot \overset{*}{\mathfrak{M}}{}^{\mathrm{T}}_{ll'} \big) \Big] \bigg)$$

where for the asterisked term we identified the matrix A as $A \equiv \mathbb{1}_5$. For the condensed incomplete Fourier transform of $\mathcal{F}\big[\mathcal{N}^{\varepsilon}_{lm|l(-m)}\big]$, $\mathcal{F}\big[\mathcal{V}^{\varepsilon}_{lm|l(-m)}\big]$ and $\mathcal{F}\big[\mathcal{W}^{\varepsilon}_{lm|l(-m)}\big]$ we proceed in precisely the same way with the slight difference that the latter two do not involve asterisked terms. In all four cases the matrix $\mathcal{Z}$ is given by

$$\mathcal{Z} = \left(\begin{array}{c|cc|c} \omega(|\vec{p}|)\omega(|\vec{q}|) & -|\vec{p}|\omega(|\vec{q}|) & \mathbf{0}_{1\times 2} & -\mu\omega(|\vec{q}|) \\ \hline -\omega(|\vec{p}|)|\vec{q}| & |\vec{p}||\vec{q}| & \mathbf{0}_{1\times 2} & \mu|\vec{q}| \\ \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 1} \\ \hline -\mu\omega(|\vec{p}|) & \mu|\vec{p}| & \mathbf{0}_{1\times 2} & \mu^2 \end{array}\right)$$

For the condensed incomplete Fourier transform of $\mathcal{F}\big[\mathcal{K}^\varepsilon_{00}\big]$ we have to identify the matrices A, B and vectors v, w as

$$A \equiv \mathfrak{C}^\varepsilon_{\mathcal{K}}, \quad B \equiv \mathfrak{K}_0 \qquad \text{and} \qquad v \equiv \mathbb{1}_{5\times 1}, \quad w \equiv \begin{pmatrix} p^0 \\ |\vec{p}| \\ 0 \\ 0 \\ \mu \end{pmatrix}$$

and thus obtain

$$\Big\{\mathcal{F}\big[\mathcal{K}^\varepsilon_{00}\big]\Big\} = \int_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0, r)\, \frac{r^2 E^\varepsilon_{\mathcal{K}}}{\sqrt{4\pi}}\, \mathrm{tr}\Big[\mathfrak{C}^\varepsilon_{\mathcal{K}}\big(\mathcal{Z}_{\mathcal{K}} \odot \mathfrak{K}_0^{\mathrm{T}}\big)\Big] \tag{F.3}$$

where the matrix $\mathcal{Z}_{\mathcal{K}}$ is given by

$$\mathcal{Z}_{\mathcal{K}} = \left(\begin{array}{c|cc|c} -\omega(|\vec{p}|) & -\omega(|\vec{p}|) & \mathbf{0}_{1\times 2} & -\omega(|\vec{p}|) \\ \hline |\vec{p}| & |\vec{p}| & \mathbf{0}_{1\times 2} & |\vec{p}| \\ \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 1} \\ \hline \mu & \mu & \mathbf{0}_{1\times 2} & \mu \end{array}\right) \tag{F.4}$$

This concludes the proof. □

By using the Hadamard product form of the condensed incomplete Fourier transforms as derived in this proposition, the integrals of the momentum-dependent parts appearing in (5.28b) can be computed more conveniently.

F.2 Momentum Integration in $\delta^2\mathcal{S}^\varepsilon$ for Lorentz Boosts

In order to demonstrate that the iε-regularized causal action is invariant under Lorentz boosts of the velocity vector of the regularization, the corresponding second variation as derived in (5.28b) has to vanish. For the sake of clarity and to streamline the proof of Lemma F.2.2, we outsourced the lengthy computations to the following preparatory proposition.

Proposition F.2.1 (Momentum Integrals for Lorentz Boosts)

Let $E^\varepsilon_{\mathcal{K}}$, $E^\varepsilon_{\mathcal{M}}$, $E^\varepsilon_{\mathcal{N}}$, $E^\varepsilon_{\mathcal{V}}$, $E^\varepsilon_{\mathcal{W}}$ be the regularization-dependent functions introduced in (4.13b), (4.19a,ii), (4.19b,ii), (4.24a,i), (4.24b,i), let $\mathcal{Z}$, $\mathcal{Z}_{\mathcal{K}}$ be the matrices from (F.2a), (F.2b) and let furthermore $\mathfrak{K}_0$, $\mathfrak{M}_{11}$, $\mathfrak{N}_{11}$, $\overset{*}{\mathfrak{M}}_{11}$, $\overset{*}{\mathfrak{N}}_{11}$ denote the first multipole matrices as explicitly given in Auxiliary Calculation E.2.1. Then the following relations hold

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}\;\omega_p \mathrm{e}^{-\varepsilon\omega_p}\;E^\varepsilon_{\mathcal{K}}\big(\mathcal{Z}_{\mathcal{K}}\odot\mathfrak{K}_0^{\mathrm{T}}\big) =$$

$$= 128\pi^2 \left(\begin{array}{c|cc|c} \mathrm{i}\Big(g-\mu^2(\xi^\varepsilon_-)^0(\xi^\varepsilon_-)^0\frac{g'}{\Xi^\varepsilon_-}\Big) & 0 & \mathbf{0}_{1\times2} & 0 \\ \hline 0 & -\mathrm{i}(\xi^\varepsilon_-)^0(\mu r)^2\frac{g'}{\Xi^\varepsilon_-} & \mathbf{0}_{1\times2} & 0 \\ \mathbf{0}_{2\times1} & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \mathbf{0}_{2\times1} \\ \hline 0 & 0 & \mathbf{0}_{1\times2} & -\mu(\xi^\varepsilon_-)^0 g \end{array}\right) \tag{F.5a}$$

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}\;|\vec{p}|^2 \mathrm{e}^{-\varepsilon\omega_p}\;E^\varepsilon_{\mathcal{K}}\big(\mathcal{Z}_{\mathcal{K}}\odot\mathfrak{K}_0^{\mathrm{T}}\big) =$$

$$= 128\pi^2 \left(\begin{array}{c|cc|c} -\mu^2(\xi^\varepsilon_-)^0\Big[3\frac{g'}{\Xi^\varepsilon_-}+\frac{(\mu r)^2}{(\Xi^\varepsilon_-)^2}\Big(g''-\frac{g'}{\Xi^\varepsilon_-}\Big)\Big] & 0 & \mathbf{0}_{1\times2} & 0 \\ \hline 0 & -\Big[5(\mu r)^2\frac{g'}{\Xi^\varepsilon_-}+\frac{(\mu r)^4}{\Xi^\varepsilon_-}\Big(g''-\frac{g'}{\Xi^\varepsilon_-}\Big)\Big] & \mathbf{0}_{1\times2} & 0 \\ \mathbf{0}_{2\times1} & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \mathbf{0}_{2\times1} \\ \hline 0 & 0 & \mathbf{0}_{1\times2} & \mathrm{i}\mu\Big(3g+(\mu r)^2\frac{g'}{\Xi^\varepsilon_-}\Big) \end{array}\right) \tag{F.5b}$$

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}|\vec{p}|\mathrm{e}^{-\varepsilon\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}|\vec{q}|\mathrm{e}^{-\varepsilon\omega_q}\;\begin{Bmatrix} E^\varepsilon_{\mathcal{M}} \\ E^\varepsilon_{\mathcal{V}} \end{Bmatrix}\big(\mathcal{Z}\odot\mathfrak{M}_{11}^{\mathrm{T}}\big) =$$

$$= 64\pi^2 \begin{Bmatrix} 1 \\ \frac{8}{\partial_r\mathcal{L}^\varepsilon(\xi)} \end{Bmatrix} \left(\begin{array}{c|cc|c} -(\mu r)^4\Big[(\xi^\varepsilon_-)^0\frac{g'}{\Xi^\varepsilon_-}\Big]^2 & -(\xi^\varepsilon_-)^0 r^2(\mu r)^2\frac{g'}{\Xi^\varepsilon_-}\Big(g+(\mu r)^2\frac{g'}{\Xi^\varepsilon_-}\Big) & \mathbf{0}_{1\times2} & \mathrm{i}(\xi^\varepsilon_-)^0 r(\mu r)^3 g\frac{g'}{\Xi^\varepsilon_-} \\ \hline -(\xi^\varepsilon_-)^0 r^2(\mu r)^2\frac{g'}{\Xi^\varepsilon_-}\Big(g_-+(\mu r)^2\frac{g'}{\Xi^\varepsilon_-}\Big) & -r^4\Big(g_-+(\mu r)^2\frac{g'}{\Xi^\varepsilon_-}\Big)^2 & \mathbf{0}_{1\times2} & \mathrm{i}r^3(\mu r)\Big(g^2+(\mu r)^2 g\frac{g'}{\Xi^\varepsilon_-}\Big) \\ \mathbf{0}_{2\times1} & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \mathbf{0}_{2\times1} \\ \hline \mathrm{i}(\xi^\varepsilon_-)^0 r(\mu r)^3 g\frac{g'}{\Xi^\varepsilon_-} & \mathrm{i}r^3(\mu r)\Big(g^2+(\mu r)^2 g\frac{g'}{\Xi^\varepsilon_-}\Big) & \mathbf{0}_{1\times2} & r^2(\mu r)^2 g^2 \end{array}\right) \tag{F.5c}$$

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}|\vec{p}|\mathrm{e}^{-\varepsilon\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}|\vec{q}|\mathrm{e}^{-\varepsilon\omega_q}\;\begin{Bmatrix} E^\varepsilon_{\mathcal{N}} \\ E^\varepsilon_{\mathcal{W}} \end{Bmatrix}\big(\mathcal{Z}\odot\mathfrak{N}_{11}^{\mathrm{T}}\big) =$$

$$= 64\pi^2 \begin{Bmatrix} 1 \\ \frac{8}{\partial_r\mathcal{L}^\varepsilon(\xi)} \end{Bmatrix} \left(\begin{array}{c|cc|c} (\mu r)^4\Big|(\xi^\varepsilon_-)^0\frac{g'}{\Xi^\varepsilon_-}\Big|^2 & (\xi^\varepsilon_+)^0 r^2(\mu r)^2\frac{\bar{g}'}{\Xi^\varepsilon_+}\Big(g+(\mu r)^2\frac{g'}{\Xi^\varepsilon_-}\Big) & \mathbf{0}_{1\times2} & -\mathrm{i}(\xi^\varepsilon_+)^0 r(\mu r)^3 g\frac{\bar{g}'}{\Xi^\varepsilon_+} \\ \hline (\xi^\varepsilon_-)^0 r^2(\mu r)^2\frac{g'}{\Xi^\varepsilon_-}\Big(\bar{g}+(\mu r)^2\frac{\bar{g}'}{\Xi^\varepsilon_+}\Big) & r^4\Big|g+(\mu r)^2\frac{g'}{\Xi^\varepsilon_-}\Big|^2 & \mathbf{0}_{1\times2} & -\mathrm{i}r^3(\mu r)\Big(|g|^2+(\mu r)^2 g\frac{\bar{g}'}{\Xi^\varepsilon_+}\Big) \\ \mathbf{0}_{2\times1} & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \mathbf{0}_{2\times1} \\ \hline \mathrm{i}(\xi^\varepsilon_-)^0 r(\mu r)^3\bar{g}\frac{g'}{\Xi^\varepsilon_-} & \mathrm{i}r^3(\mu r)\Big(|g|^2+(\mu r)^2\bar{g}\frac{g'}{\Xi^\varepsilon_-}\Big) & \mathbf{0}_{1\times2} & (mr^2)^2|g|^2 \end{array}\right) \tag{F.5d}$$

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}|\vec{p}|\mathrm{e}^{-\varepsilon\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}|\vec{q}|\mathrm{e}^{-\varepsilon\omega_q}\;E^\varepsilon_{\mathcal{M}}\big(\mathcal{Z}\odot\overset{*}{\mathfrak{M}}{}_{11}^{\mathrm{T}}\big) =$$

$$= 64\pi^2 \left(\begin{array}{c|cc|c} 0 & 0 & \mathbf{0}_{1\times2} & 0 \\ \hline 0 & -3g^2-2(\mu r)^2 g\frac{g'}{\Xi^\varepsilon_-}-(\mu r)^4\Big(\frac{g'}{\Xi^\varepsilon_-}\Big)^2 & \mathbf{0}_{1\times2} & 0 \\ \mathbf{0}_{2\times1} & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \mathbf{0}_{2\times1} \\ \hline 0 & 0 & \mathbf{0}_{1\times2} & 0 \end{array}\right) \tag{F.5e}$$

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}|\vec{p}|\mathrm{e}^{-\varepsilon\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}|\vec{q}|\mathrm{e}^{-\varepsilon\omega_q}\;E^\varepsilon_{\mathcal{N}}\big(\mathcal{Z}\odot\overset{*}{\mathfrak{N}}{}_{11}^{\mathrm{T}}\big) =$$

$$= 64\pi^2 \left(\begin{array}{c|cc|c} 0 & 0 & \mathbf{0}_{1\times2} & 0 \\ \hline 0 & 3|g|^2+2(\mu r)^2\,\mathrm{Re}\Big[\bar{g}\frac{g'}{\Xi^\varepsilon_-}\Big]+(\mu r)^2\Big|\frac{g'}{\Xi^\varepsilon_-}\Big|^2 & \mathbf{0}_{1\times2} & 0 \\ \mathbf{0}_{2\times1} & \mathbf{0}_{2\times1} & \mathbf{0}_{2\times2} & \mathbf{0}_{2\times1} \\ \hline 0 & 0 & \mathbf{0}_{1\times2} & 0 \end{array}\right) \tag{F.5f}$$

Proof. To prove the stated relations, we make use of the Hadamard product form of the condensed incomplete Fourier transforms as given in Proposition F.1.1 and consider the different terms separately.

(1) Expressions containing $\mathfrak{K}_0$
We start by evaluating the simplest expression, namely the one containing $\mathfrak{K}_0$. Inserting the definition of the matrix $\mathcal{Z}_{\mathcal{K}}$ from (F.2b), the explicit form of the function $E^\varepsilon_{\mathcal{K}}$ from (4.13b) as well as the matrix $\mathfrak{K}_0$ from (E.1a), we obtain

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}\,\omega_p \mathrm{e}^{-\varepsilon\omega_p}\; E^\varepsilon_{\mathcal{K}}\big(\mathcal{Z}_{\mathcal{K}} \odot \mathfrak{K}_0^{\mathrm{T}}\big) =$$

$$\overset{(4.13b)}{\underset{(F.2a)}{=}} 256\pi^2 \int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}\,\frac{\omega_p \mathrm{e}^{-(\varepsilon+\mathrm{i}\xi^0)\omega_p}}{2\omega_p} \left(\begin{array}{c|cc|c} -\omega(|\vec{p}|) & -\omega(|\vec{p}|) & \mathbf{0}_{1\times 2} & -\omega(|\vec{p}|) \\ \hline |\vec{p}| & |\vec{p}| & \mathbf{0}_{1\times 2} & |\vec{p}| \\ \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 1} \\ \hline \mu & \mu & \mathbf{0}_{1\times 2} & \mu \end{array}\right) \odot$$

$$\odot \left[\mathrm{diag}\Big(0, \frac{\mathrm{i}}{|\vec{p}|}, 0, 0, 0\Big)\cos(|\vec{p}|r) + \mathrm{diag}\Big(1, -\frac{\mathrm{i}}{|\vec{p}|}, 0, 0, 1\Big)\frac{\sin(|\vec{p}|r)}{|\vec{p}|r}\right]$$

Carrying out the Hadamard product yields

$$\cdots = 128\pi^2 \int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}\,\mathrm{e}^{-(\varepsilon+\mathrm{i}\xi^0)\omega_p} \Big[\mathrm{diag}\big(0, \mathrm{i}, 0, 0, 0\big)\cos(|\vec{p}|r) + \mathrm{diag}\big(-\omega_p, -\mathrm{i}, 0, 0, \mu\big)\frac{\sin(|\vec{p}|r)}{|\vec{p}|r}\Big]$$

Having arrived at this point, the integral can be computed explicitly using the corresponding relation from Corollary A.2.3. Simplifying the resulting expression by cancelling and combining terms results in

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}\,\omega_p \mathrm{e}^{-\varepsilon\omega_p}\; E^\varepsilon_{\mathcal{K}}\big(\mathcal{Z}_{\mathcal{K}} \odot \mathfrak{K}_0^{\mathrm{T}}\big) =$$

$$\overset{(A.12)}{=} 128\pi^2 \left(\begin{array}{c|cc|c} \mathrm{i}\Big(g - \mu^2(\xi^\varepsilon_-)^0(\xi^\varepsilon_-)^0\frac{g'}{\Xi^\varepsilon_-}\Big) & 0 & \mathbf{0}_{1\times 2} & 0 \\ \hline 0 & -\mathrm{i}(\xi^\varepsilon_-)^0(\mu r)^2\frac{g'}{\Xi^\varepsilon_-} & \mathbf{0}_{1\times 2} & 0 \\ \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 1} \\ \hline 0 & 0 & \mathbf{0}_{1\times 2} & -\mu(\xi^\varepsilon_-)^0 g \end{array}\right)$$

For the same integral with the factor ω_p replaced by two more powers of $|\vec{p}|$ in the integrand, we analogously find the following similar, though slightly more complicated expression

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}\,|\vec{p}|^2 \mathrm{e}^{-\varepsilon\omega_p}\; E^\varepsilon_{\mathcal{K}}\big(\mathcal{Z}_{\mathcal{K}} \odot \mathfrak{K}_0^{\mathrm{T}}\big) =$$

$$\overset{(A.12)}{=} 128\pi^2 \left(\begin{array}{c|cc|c} -\mu^2(\xi^\varepsilon_-)^0\Big[3\frac{g'}{\Xi^\varepsilon_-} + \frac{(\mu r)^2}{(\Xi^\varepsilon_-)^2}\Big(g'' - \frac{g'}{\Xi^\varepsilon_-}\Big)\Big] & 0 & \mathbf{0}_{1\times 2} & 0 \\ \hline 0 & -\Big[5(\mu r)^2\frac{g'}{\Xi^\varepsilon_-} + \frac{(\mu r)^4}{\Xi^\varepsilon_-}\Big(g'' - \frac{g'}{\Xi^\varepsilon_-}\Big)\Big] & \mathbf{0}_{1\times 2} & 0 \\ \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 1} \\ \hline 0 & 0 & \mathbf{0}_{1\times 2} & \mathrm{i}\mu\Big(3g + (\mu r)^2\frac{g'}{\Xi^\varepsilon_-}\Big) \end{array}\right) \tag{F.6}$$

(2) Expressions containing $\mathfrak{M}_{11}$ and $\mathfrak{N}_{11}$
Next, we consider terms which contain the multipole matrices $\mathfrak{M}_{11}$ and $\mathfrak{N}_{11}$, respectively.

(a) Terms containing $\mathfrak{M}_{11}$

Inserting the definition of the matrix $\mathcal{Z}$ from (F.2b) (with zero rows and columns suppressed), the explicit form of the function $E^\varepsilon_{\mathcal{M}}$ from (4.19a,ii) as well as the matrix $\mathfrak{M}_{11}$ from (E.3a) (again, with zero rows and columns suppressed), we obtain

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}|\vec{p}|\mathrm{e}^{-\varepsilon\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}|\vec{q}|\mathrm{e}^{-\varepsilon\omega_q}\left\{\begin{matrix}E^\varepsilon_{\mathcal{M}}\\ E^\varepsilon_{\mathcal{V}}\end{matrix}\right\}\left(\mathcal{Z}\odot\mathfrak{M}^{\mathrm{T}}_{11}\right) =$$

$$\overset{(4.19\mathrm{a,ii})}{\underset{(\mathrm{F.2b})}{=}} 256\pi^2\left\{\begin{matrix}1\\ \frac{8}{\partial_r\mathcal{L}^\varepsilon(\xi)}\end{matrix}\right\}\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}\frac{|\vec{p}|\mathrm{e}^{-(\varepsilon+\mathrm{i}\xi^0)\omega_p}}{2\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}\frac{|\vec{q}|\mathrm{e}^{-(\varepsilon+\mathrm{i}\xi^0)\omega_q}}{2\omega_q}\times$$

$$\times\begin{pmatrix}\omega(|\vec{p}|)\omega(|\vec{q}|) & -|\vec{p}|\omega(|\vec{q}|) & -\mu\omega(|\vec{q}|)\\ -\omega(|\vec{p}|)|\vec{q}| & |\vec{p}||\vec{q}| & \mu|\vec{q}|\\ -\mu\omega(|\vec{p}|) & \mu|\vec{p}| & \mu^2\end{pmatrix}\odot\left[\begin{pmatrix}-1 & 2\frac{\mathrm{i}}{|\vec{p}|} & -1\\ 2\frac{\mathrm{i}}{|\vec{q}|} & 4\frac{1}{|\vec{p}||\vec{q}|} & 2\frac{\mathrm{i}}{|\vec{q}|}\\ -1 & 2\frac{\mathrm{i}}{|\vec{p}|} & -1\end{pmatrix}\frac{\cos(|\vec{p}|r)}{|\vec{p}|r}\frac{\cos(|\vec{q}|r)}{|\vec{q}|r}\right.$$

$$+\begin{pmatrix}-1 & [2-(|\vec{p}|r)^2]\frac{\mathrm{i}}{|\vec{p}|} & -1\\ [2-(|\vec{q}|r)^2]\frac{\mathrm{i}}{|\vec{q}|} & [2-(|\vec{p}|r)^2][2-(|\vec{q}|r)^2]\frac{1}{|\vec{p}||\vec{q}|} & [2-(|\vec{q}|r)^2]\frac{\mathrm{i}}{|\vec{q}|}\\ -1 & [2-(|\vec{p}|r)^2]\frac{\mathrm{i}}{|\vec{p}|} & -1\end{pmatrix}\frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^2}\frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^2}$$

$$+\begin{pmatrix}1 & -[2-(|\vec{p}|r)^2]\frac{\mathrm{i}}{|\vec{p}|} & 1\\ -2\frac{\mathrm{i}}{|\vec{q}|} & -2[2-(|\vec{p}|r)^2]\frac{1}{|\vec{p}||\vec{q}|} & -2\frac{\mathrm{i}}{|\vec{q}|}\\ 1 & -[2-(|\vec{p}|r)^2]\frac{\mathrm{i}}{|\vec{p}|} & 1\end{pmatrix}\frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^2}\frac{\cos(|\vec{q}|r)}{|\vec{q}|r}$$

$$\left.+\begin{pmatrix}1 & -2\frac{\mathrm{i}}{|\vec{p}|} & 1\\ -[2-(|\vec{q}|r)^2]\frac{\mathrm{i}}{|\vec{q}|} & -2[2-(|\vec{q}|r)^2]\frac{1}{|\vec{p}||\vec{q}|} & -[2-(|\vec{q}|r)^2]\frac{\mathrm{i}}{|\vec{q}|}\\ 1 & -2\frac{\mathrm{i}}{|\vec{p}|} & 1\end{pmatrix}\frac{\cos(|\vec{p}|r)}{|\vec{p}|r}\frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^2}\right]$$

Carrying out the remaining Hadamard products and factoring out powers of r, we find

$$\cdots = 64\pi^2\left\{\begin{matrix}1\\ \frac{8}{\partial_r\mathcal{L}^\varepsilon(\xi)}\end{matrix}\right\}\int_0^\infty \frac{\mathrm{d}|\vec{p}|}{(2\pi)^3}\frac{\mathrm{e}^{-(\varepsilon+\mathrm{i}\xi^0)\omega_p}}{\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|}{(2\pi)^3}\frac{\mathrm{e}^{-(\varepsilon+\mathrm{i}\xi^0)\omega_q}}{\omega_q}\times$$

$$\times\left[\frac{1}{r^2}\begin{pmatrix}-\omega_p\omega_q & -2\mathrm{i}\omega_q & \mu\omega_q\\ -2\mathrm{i}\omega_p & 4 & 2\mathrm{i}\mu\\ \mu\omega_p & 2\mathrm{i}\mu & -\mu^2\end{pmatrix}|\vec{p}|^2\cos(|\vec{p}|r)|\vec{q}|^2\cos(|\vec{q}|r)\right.$$

$$+\frac{1}{r^4}\begin{pmatrix}-\omega_p\omega_q & -\mathrm{i}[2-(|\vec{p}|r)^2]\omega_q & \mu\omega_q\\ -\mathrm{i}\omega_p[2-(|\vec{q}|r)^2] & [2-(|\vec{p}|r)^2][2-(|\vec{q}|r)^2] & \mathrm{i}\mu[2-(|\vec{q}|r)^2]\\ \mu\omega_p & \mathrm{i}\mu[2-(|\vec{p}|r)^2] & -\mu^2\end{pmatrix}|\vec{p}|\sin(|\vec{p}|r)|\vec{q}|\sin(|\vec{q}|r)$$

$$+\frac{1}{r^3}\begin{pmatrix}\omega_p\omega_q & \mathrm{i}[2-(|\vec{p}|r)^2]\omega_q & -\mu\omega_q\\ 2\mathrm{i}\omega_p & -2[2-(|\vec{p}|r)^2] & -2\mathrm{i}\mu\\ -\mu\omega_p & -\mathrm{i}\mu[2-(|\vec{p}|r)^2] & \mu^2\end{pmatrix}|\vec{p}|\sin(|\vec{p}|r)|\vec{q}|^2\cos(|\vec{q}|r)$$

$$\left.+\frac{1}{r^3}\begin{pmatrix}\omega_p\omega_q & 2\mathrm{i}\omega_q & -\mu\omega_q\\ \mathrm{i}\omega_p[2-(|\vec{q}|r)^2] & -2[2-(|\vec{q}|r)^2] & -\mathrm{i}\mu[2-(|\vec{q}|r)^2]\\ -\mu\omega_p & -2\mathrm{i}\mu & \mu^2\end{pmatrix}|\vec{p}|^2\cos(|\vec{p}|r)|\vec{q}|\sin(|\vec{q}|r)\right]$$

Having arrived at this point, the integrals can by computed explicitly using the relations from Corollary A.2.3. Simplifying the resulting expression by cancelling and combining terms and restoring the zero rows and columns results in

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}|\vec{p}|\mathrm{e}^{-\varepsilon\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}|\vec{q}|\mathrm{e}^{-\varepsilon\omega_q}\left\{\begin{matrix}E^\varepsilon_{\mathcal{M}}\\ E^\varepsilon_{\mathcal{V}}\end{matrix}\right\}\left(\mathcal{Z}\odot\mathfrak{M}^{\mathrm{T}}_{11}\right) =$$

$$\overset{\text{(A.12)}}{=} 64\pi^2 \left\{ \begin{matrix} 1 \\ \frac{8}{\partial_r \mathcal{L}^\varepsilon(\xi)} \end{matrix} \right\} \left(\begin{array}{c|cc|c} -(\mu r)^4\left[(\xi_-^\varepsilon)^0 \frac{g'}{\Xi_-^\varepsilon}\right]^2 & -(\xi_-^\varepsilon)^0 r^2(\mu r)^2 \frac{g'}{\Xi_-^\varepsilon}\left(g + (\mu r)^2 \frac{g'}{\Xi_-^\varepsilon}\right) & \mathbf{0}_{1\times 2} & \mathrm{i}(\xi_-^\varepsilon)^0 r(\mu r)^3 g \frac{g'}{\Xi_-^\varepsilon} \\ \hline -(\xi_-^\varepsilon)^0 r^2(\mu r)^2 \frac{g'}{\Xi_-^\varepsilon}\left(g_- + (\mu r)^2 \frac{g'}{\Xi_-^\varepsilon}\right) & -r^4\left(g_- + (\mu r)^2 \frac{g'}{\Xi_-^\varepsilon}\right)^2 & \mathbf{0}_{1\times 2} & \mathrm{i}r^3(\mu r)\left(g^2 + (\mu r)^2 g \frac{g'}{\Xi_-^\varepsilon}\right) \\ \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 1} \\ \hline \mathrm{i}(\xi_-^\varepsilon)^0 r(\mu r)^3 g \frac{g'}{\Xi_-^\varepsilon} & \mathrm{i}r^3(\mu r)\left(g^2 + (\mu r)^2 g \frac{g'}{\Xi_-^\varepsilon}\right) & \mathbf{0}_{1\times 2} & r^2(\mu r)^2 g^2 \end{array} \right)$$

(b) Terms containing $\mathfrak{N}_{11}$

For terms containing $\mathfrak{N}_{11}$ we basically proceed in the same way as before, though with a slight difference: As a consequence of different signs in the exponential factors contained in the function $E^\varepsilon_{\mathcal{N}}$ compared with $E^\varepsilon_{\mathcal{M}}$ as well as the different form of the matrix $\mathfrak{N}_{11}$ itself, we will end up with a different matrix in comparison to the previous result. Inserting the definition of the matrix $\mathcal{Z}$ from (F.2b) (with zero rows and columns suppressed), the explicit form of the function $E^\varepsilon_{\mathcal{N}}$ from (4.19b,ii) as well as the matrix $\mathfrak{N}_{11}$ from (E.3b) (again, with zero rows and columns suppressed), we obtain

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}|\vec{p}|\mathrm{e}^{-\varepsilon\omega_p} \int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}|\vec{q}|\mathrm{e}^{-\varepsilon\omega_q} \left\{ \begin{matrix} E^\varepsilon_{\mathcal{N}} \\ E^\varepsilon_{\mathcal{W}} \end{matrix} \right\} \left(\mathcal{Z} \odot \mathfrak{N}_{11}^{\mathrm{T}}\right) =$$

$$\overset{\text{(4.19b,ii)}}{\underset{\text{(F.2b)}}{=}} 256\pi^2 \left\{ \begin{matrix} 1 \\ \frac{8}{\partial_r \mathcal{L}^\varepsilon(\xi)} \end{matrix} \right\} \int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3} \frac{|\vec{p}|\mathrm{e}^{-(\varepsilon+\mathrm{i}\xi^0)\omega_p}}{2\omega_p} \int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3} \frac{|\vec{q}|\mathrm{e}^{-(\varepsilon-\mathrm{i}\xi^0)\omega_q}}{2\omega_q} \times$$

$$\times \begin{pmatrix} \omega(|\vec{p}|)\omega(|\vec{q}|) & -|\vec{p}|\omega(|\vec{q}|) & -\mu\omega(|\vec{q}|) \\ -\omega(|\vec{p}|)|\vec{q}| & |\vec{p}||\vec{q}| & \mu|\vec{q}| \\ -\mu\omega(|\vec{p}|) & \mu|\vec{p}| & \mu^2 \end{pmatrix} \odot \left[\begin{pmatrix} 1 & -2\frac{\mathrm{i}}{|\vec{p}|} & 1 \\ 2\frac{\mathrm{i}}{|\vec{q}|} & 4\frac{1}{|\vec{p}||\vec{q}|} & 2\frac{\mathrm{i}}{|\vec{q}|} \\ 1 & -2\frac{\mathrm{i}}{|\vec{p}|} & 1 \end{pmatrix} \frac{\cos(|\vec{p}|r)}{|\vec{p}|r}\frac{\cos(|\vec{q}|r)}{|\vec{q}|r} \right.$$

$$+ \begin{pmatrix} 1 & -\left[2-(|\vec{p}|r)^2\right]\frac{\mathrm{i}}{|\vec{p}|} & 1 \\ \left[2-(|\vec{q}|r)^2\right]\frac{\mathrm{i}}{|\vec{q}|} & \left[2-(|\vec{p}|r)^2\right]\left[2-(|\vec{q}|r)^2\right]\frac{1}{|\vec{p}||\vec{q}|} & \left[2-(|\vec{q}|r)^2\right]\frac{\mathrm{i}}{|\vec{q}|} \\ 1 & -\left[2-(|\vec{p}|r)^2\right]\frac{\mathrm{i}}{|\vec{p}|} & 1 \end{pmatrix} \frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^2}\frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^2}$$

$$+ \begin{pmatrix} -1 & \left[2-(|\vec{p}|r)^2\right]\frac{\mathrm{i}}{|\vec{p}|} & -1 \\ -2\frac{\mathrm{i}}{|\vec{q}|} & -2\left[2-(|\vec{p}|r)^2\right]\frac{1}{|\vec{p}||\vec{q}|} & -2\frac{\mathrm{i}}{|\vec{q}|} \\ -1 & \left[2-(|\vec{p}|r)^2\right]\frac{\mathrm{i}}{|\vec{p}|} & -1 \end{pmatrix} \frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^2}\frac{\cos(|\vec{q}|r)}{|\vec{q}|r}$$

$$\left. + \begin{pmatrix} -1 & 2\frac{\mathrm{i}}{|\vec{p}|} & -1 \\ -\left[2-(|\vec{q}|r)^2\right]\frac{\mathrm{i}}{|\vec{q}|} & -2\left[2-(|\vec{q}|r)^2\right]\frac{1}{|\vec{p}||\vec{q}|} & -\left[2-(|\vec{q}|r)^2\right]\frac{\mathrm{i}}{|\vec{q}|} \\ -1 & 2\frac{\mathrm{i}}{|\vec{p}|} & -1 \end{pmatrix} \frac{\cos(|\vec{p}|r)}{|\vec{p}|r}\frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^2} \right]$$

Carrying out the remaining Hadamard products and factoring out powers of r, we find

$$\cdots = 64\pi^2 \left\{ \begin{matrix} 1 \\ \frac{8}{\partial_r \mathcal{L}^\varepsilon(\xi)} \end{matrix} \right\} \int_0^\infty \frac{\mathrm{d}|\vec{p}|}{(2\pi)^3} \frac{\mathrm{e}^{-(\varepsilon+\mathrm{i}\xi^0)\omega_p}}{\omega_p} \int_0^\infty \frac{\mathrm{d}|\vec{q}|}{(2\pi)^3} \frac{\mathrm{e}^{-(\varepsilon-\mathrm{i}\xi^0)\omega_q}}{\omega_q} \times$$

$$\times \left[\frac{1}{r^2} \begin{pmatrix} \omega_p\omega_q & 2\mathrm{i}\omega_q & -\mu\omega_q \\ -2\mathrm{i}\omega_p & 4 & 2\mathrm{i}\mu \\ -\mu\omega_p & -2\mathrm{i}\mu & \mu^2 \end{pmatrix} |\vec{p}|^2\cos(|\vec{p}|r)|\vec{q}|^2\cos(|\vec{q}|r) \right.$$

$$+ \frac{1}{r^4} \begin{pmatrix} \omega_p\omega_q & \mathrm{i}\left[2-(|\vec{p}|r)^2\right]\omega_q & -\mu\omega_q \\ -\mathrm{i}\omega_p\left[2-(|\vec{q}|r)^2\right] & \left[2-(|\vec{p}|r)^2\right]\left[2-(|\vec{q}|r)^2\right] & \mathrm{i}\mu\left[2-(|\vec{q}|r)^2\right] \\ -\mu\omega_p & -\mathrm{i}\mu\left[2-(|\vec{p}|r)^2\right] & \mu^2 \end{pmatrix} |\vec{p}|\sin(|\vec{p}|r)|\vec{q}|\sin(|\vec{q}|r)$$

$$+ \frac{1}{r^3} \begin{pmatrix} -\omega_p\omega_q & -\mathrm{i}\left[2-(|\vec{p}|r)^2\right]\omega_q & \mu\omega_q \\ 2\mathrm{i}\omega_p & -2\left[2-(|\vec{p}|r)^2\right] & -2\mathrm{i}\mu \\ \mu\omega_p & \mathrm{i}\mu\left[2-(|\vec{p}|r)^2\right] & -\mu^2 \end{pmatrix} |\vec{p}|\sin(|\vec{p}|r)|\vec{q}|^2\cos(|\vec{q}|r)$$

$$\left. + \frac{1}{r^3} \begin{pmatrix} -\omega_p\omega_q & -2\mathrm{i}\omega_q & \mu\omega_q \\ \mathrm{i}\omega_p\left[2-(|\vec{q}|r)^2\right] & -2\left[2-(|\vec{q}|r)^2\right] & -\mathrm{i}\mu\left[2-(|\vec{q}|r)^2\right] \\ \mu\omega_p & 2\mathrm{i}\mu & -\mu^2 \end{pmatrix} |\vec{p}|^2\cos(|\vec{p}|r)|\vec{q}|\sin(|\vec{q}|r) \right]$$

Having arrived at this point, the integrals can by computed explicitly using the relations from Corollary A.2.3. Simplifying the resulting expression by cancelling and combining terms and restoring zero rows and columns finally results in

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}|\vec{p}|\mathrm{e}^{-\varepsilon\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}|\vec{q}|\mathrm{e}^{-\varepsilon\omega_q}\;\begin{Bmatrix} E^\varepsilon_{\mathcal{N}} \\ E^\varepsilon_{\mathcal{W}}\end{Bmatrix}\left(\mathcal{Z}\odot\mathfrak{N}^{\mathrm{T}}_{11}\right) =$$

$$\overset{(A.12)}{=} 64\pi^2\begin{Bmatrix} 1 \\ \frac{8}{\partial_r\mathcal{L}^\varepsilon(\xi)}\end{Bmatrix}\left(\begin{array}{c|cc|c} (\mu r)^4\left|(\xi^\varepsilon_-)^0\frac{g'}{\Xi^\varepsilon_-}\right|^2 & (\xi^\varepsilon_+)^0 r^2(\mu r)^2\frac{\bar{g}'}{\Xi^\varepsilon_+}\left(g+(\mu r)^2\frac{g'}{\Xi^\varepsilon_-}\right) & \mathbf{0}_{1\times 2} & -\mathrm{i}(\xi^\varepsilon_+)^0 r(\mu r)^3 g\frac{\bar{g}'}{\Xi^\varepsilon_+} \\ \hline (\xi^\varepsilon_-)^0 r^2(\mu r)^2\frac{g'}{\Xi^\varepsilon_-}\left(\bar{g}+(\mu r)^2\frac{\bar{g}'}{\Xi^\varepsilon_+}\right) & r^4\left|g+(\mu r)^2\frac{g'}{\Xi^\varepsilon_-}\right|^2 & \mathbf{0}_{1\times 2} & -\mathrm{i}r^3(\mu r)\left(|g|^2+(\mu r)^2 g\frac{\bar{g}'}{\Xi^\varepsilon_+}\right) \\ \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 1} \\ \hline \mathrm{i}(\xi^\varepsilon_-)^0 r(\mu r)^3\bar{g}\frac{g'}{\Xi^\varepsilon_-} & \mathrm{i}r^3(\mu r)\left(|g|^2+(\mu r)^2\bar{g}\frac{g'}{\Xi^\varepsilon_-}\right) & \mathbf{0}_{1\times 2} & (mr^2)^2|g|^2 \end{array}\right)$$

(3) Asterisked Terms

Having completed the calculation for terms without asterisks, we now turn to the computation of terms carrying asterisks.

(a) Terms containing $\overset{*}{\mathcal{M}}_{11}$

Inserting the definition of the matrix $\mathcal{Z}$ from (F.2b) (with zero rows and columns suppressed), the explicit form of the function $E^\varepsilon_{\mathcal{M}}$ from (4.19a,ii) as well as the matrix $\overset{*}{\mathfrak{M}}_{11}$ from (E.3c) (again, with zero rows and columns suppressed), we obtain

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}|\vec{p}|\mathrm{e}^{-\varepsilon\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}|\vec{q}|\mathrm{e}^{-\varepsilon\omega_q}\;E^\varepsilon_{\mathcal{M}}\left(\mathcal{Z}\odot\overset{*}{\mathfrak{M}}{}^{\mathrm{T}}_{11}\right) =$$

$$\overset{(4.19a,ii)}{\underset{(F.2b)}{=}} 64\pi^2\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}\frac{|\vec{p}|\mathrm{e}^{-(\varepsilon+\mathrm{i}\xi^0)\omega_p}}{2\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}\frac{|\vec{q}|\mathrm{e}^{-(\varepsilon+\mathrm{i}\xi^0)\omega_q}}{2\omega_q}\times$$

$$\times\begin{pmatrix} \omega(|\vec{p}|)\omega(|\vec{q}|) & -|\vec{p}|\omega(|\vec{q}|) & -\mu\omega(|\vec{q}|) \\ -\omega(|\vec{p}|)|\vec{q}| & |\vec{p}||\vec{q}| & \mu|\vec{q}| \\ -\mu\omega(|\vec{p}|) & \mu|\vec{p}| & \mu^2\end{pmatrix}\odot\Bigg[\mathrm{diag}\big(0,24,0,0,0\big)\frac{\cos(|\vec{p}|r)}{(|\vec{p}|r)^2}\frac{\cos(|\vec{q}|r)}{(|\vec{q}|r)^2}$$

$$+\,\mathrm{diag}\Big(0,4\big[6-2\big((|\vec{p}|r)^2+(|\vec{q}|r)^2\big)+(|\vec{p}|r)^2(|\vec{q}|r)^2\big],0,0,0\Big)\frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^3}\frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^3}$$

$$+\,\mathrm{diag}\Big(0,-8\big[3-(|\vec{p}|r)^2\big],0,0,0\Big)\frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^3}\frac{\cos(|\vec{q}|r)}{(|\vec{q}|r)^2}$$

$$+\mathrm{diag}\Big(0,-8\big[3-(|\vec{q}|r)^2\big]\frac{1}{|\vec{p}||\vec{q}|},0,0,0\Big)\frac{\cos(|\vec{p}|r)}{(|\vec{p}|r)^2}\frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^3}\Bigg]$$

Carrying out the remaining Hadamard product and factoring out powers of r we find

$$\cdots = 16\pi^2\int_0^\infty \frac{\mathrm{d}|\vec{p}|}{(2\pi)^3}\frac{\mathrm{e}^{-(\varepsilon+\mathrm{i}\xi^0)\omega_p}}{\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|}{(2\pi)^3}\frac{\mathrm{e}^{-(\varepsilon+\mathrm{i}\xi^0)\omega_q}}{\omega_q}\times$$

$$\times\Bigg[\frac{1}{r^4}\mathrm{diag}\big(0,24,0,0,0\big)|\vec{p}|^2\cos(|\vec{p}|r)|\vec{q}|^2\cos(|\vec{q}|r)$$

$$+\,\frac{1}{r^6}\mathrm{diag}\Big(0,4\big[6-2\big((|\vec{p}|r)^2+(|\vec{q}|r)^2\big)+(|\vec{p}|r)^2(|\vec{q}|r)^2\big],0,0,0\Big)|\vec{p}|\sin(|\vec{p}|r)|\vec{q}|\sin(|\vec{q}|r)$$

$$+\,\frac{1}{r^5}\mathrm{diag}\Big(0,-8\big[3-(|\vec{p}|r)^2\big],0,0,0\Big)|\vec{p}|\sin(|\vec{p}|r)|\vec{q}|^2\cos(|\vec{q}|r)$$

$$+\frac{1}{r^5}\mathrm{diag}\Big(0,-8\big[3-(|\vec{q}|r)^2\big],0,0,0\Big)|\vec{p}|^2\cos(|\vec{p}|r)|\vec{q}|\sin(|\vec{q}|r)\Bigg]$$

Having arrived at this point, the integrals can by computed explicitly using the relations from Corollary A.2.3. Simplifying the resulting expression by cancelling and combining terms and restoring zero rows and columns results in

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}|\vec{p}|\mathrm{e}^{-\varepsilon\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}|\vec{q}|\mathrm{e}^{-\varepsilon\omega_q}\;E^\varepsilon_{\mathcal{M}}\big(\mathcal{Z}\odot\overset{*}{\mathfrak{M}}{}^{\mathrm{T}}_{11}\big) =$$

$$\overset{\text{(A.12)}}{=} 64\pi^2\left(\begin{array}{c|ccc|c} 0 & 0 & & \mathbf{0}_{1\times2} & 0 \\ \hline 0 & -3g^2-2(\mu r)^2 g\frac{g'}{\Xi^\varepsilon_-}-(\mu r)^4\Big(\frac{g'}{\Xi^\varepsilon_-}\Big)^2 & & \mathbf{0}_{1\times2} & 0 \\ \mathbf{0}_{2\times1} & \mathbf{0}_{2\times1} & & \mathbf{0}_{2\times2} & \mathbf{0}_{2\times1} \\ \hline 0 & 0 & & \mathbf{0}_{1\times2} & 0 \end{array}\right)$$

(b) Terms containing $\overset{*}{\mathcal{N}}_{11}$

Inserting the definition of the matrix $\mathcal{Z}$ from (F.2b) (with zero rows and columns suppressed), the explicit form of the function $E^\varepsilon_{\mathcal{N}}$ from (4.19b,ii) as well as the matrix $\overset{*}{\mathfrak{N}}_{11}$ from (E.3d) (again, with zero rows and columns suppressed), we obtain

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}|\vec{p}|\mathrm{e}^{-\varepsilon\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}|\vec{q}|\mathrm{e}^{-\varepsilon\omega_q}\;E^\varepsilon_{\mathcal{N}}\big(\mathcal{Z}\odot\overset{*}{\mathfrak{N}}{}^{\mathrm{T}}_{11}\big) =$$

$$\overset{(4.19\text{b,ii})}{\underset{(\text{F.2b})}{=}} 64\pi^2\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}\frac{|\vec{p}|\mathrm{e}^{-(\varepsilon+\mathrm{i}\xi^0)\omega_p}}{2\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}\frac{|\vec{q}|\mathrm{e}^{-(\varepsilon-\mathrm{i}\xi^0)\omega_q}}{2\omega_q}\begin{pmatrix} \omega(|\vec{p}|)\omega(|\vec{q}|) & -|\vec{p}|\omega(|\vec{q}|) & -\mu\omega(|\vec{q}|) \\ -\omega(|\vec{p}|)|\vec{q}| & |\vec{p}||\vec{q}| & \mu|\vec{q}| \\ -\mu\omega(|\vec{p}|) & \mu|\vec{p}| & \mu^2 \end{pmatrix}\odot$$

$$\odot\Bigg[\mathrm{diag}\big(0,24,0,0,0\big)\frac{\cos(|\vec{p}|r)}{(|\vec{p}|r)^2}\frac{\cos(|\vec{q}|r)}{(|\vec{q}|r)^2}$$

$$+\,\mathrm{diag}\Big(0,4\big[6-2\big((|\vec{p}|r)^2+(|\vec{q}|r)^2\big)+(|\vec{p}|r)^2(|\vec{q}|r)^2\big],0,0,0\Big)\frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^3}\frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^3}$$

$$+\,\mathrm{diag}\Big(0,-8\big[3-(|\vec{p}|r)^2\big],0,0,0\Big)\frac{\sin(|\vec{p}|r)}{(|\vec{p}|r)^3}\frac{\cos(|\vec{q}|r)}{(|\vec{q}|r)^2}$$

$$+\mathrm{diag}\Bigg(0,-8\big[3-(|\vec{q}|r)^2\big]\frac{1}{|\vec{p}||\vec{q}|},0,0,0\Bigg)\frac{\cos(|\vec{p}|r)}{(|\vec{p}|r)^2}\frac{\sin(|\vec{q}|r)}{(|\vec{q}|r)^3}\Bigg]$$

Carrying out the remaining Hadamard product and factoring out powers of r we find

$$\cdots = 64\pi^2\int_0^\infty \frac{\mathrm{d}|\vec{p}|}{(2\pi)^3}\frac{\mathrm{e}^{-(\varepsilon+\mathrm{i}\xi^0)\omega_p}}{2\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|}{(2\pi)^3}\frac{\mathrm{e}^{-(\varepsilon-\mathrm{i}\xi^0)\omega_q}}{2\omega_q}\times$$

$$\times\Bigg[\frac{1}{r^4}\mathrm{diag}\big(0,24,0,0,0\big)|\vec{p}|^2\cos(|\vec{p}|r)|\vec{q}|^2\cos(|\vec{q}|r)$$

$$+\,\frac{1}{r^6}\mathrm{diag}\Big(0,4\big[6-2\big((|\vec{p}|r)^2+(|\vec{q}|r)^2\big)+(|\vec{p}|r)^2(|\vec{q}|r)^2\big],0,0,0\Big)|\vec{p}|\sin(|\vec{p}|r)|\vec{q}|\sin(|\vec{q}|r)$$

$$+\,\frac{1}{r^5}\mathrm{diag}\Big(0,-8\big[3-(|\vec{p}|r)^2\big],0,0,0\Big)|\vec{p}|\sin(|\vec{p}|r)|\vec{q}|^2\cos(|\vec{q}|r)$$

$$+\frac{1}{r^5}\mathrm{diag}\Bigg(0,-8\big[3-(|\vec{q}|r)^2\big],0,0,0\Bigg)|\vec{p}|^2\cos(|\vec{p}|r)|\vec{q}|\sin(|\vec{q}|r)\Bigg]$$

Having arrived at this point, the integrals can by computed explicitly using the relations from Corollary A.2.3. Simplifying the resulting expression by cancelling and combining terms and restoring zero rows and columns results in

$$\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}|\vec{p}|\mathrm{e}^{-\varepsilon\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^3}|\vec{q}|\mathrm{e}^{-\varepsilon\omega_q}\;E^\varepsilon_{\mathcal{N}}\big(\mathcal{Z}\odot\overset{*}{\mathfrak{N}}{}^{\mathrm{T}}_{11}\big) =$$

$$\overset{\text{(A.12)}}{=} 64\pi^2 \left(\begin{array}{c|cc|c} 0 & 0 & \mathbf{0}_{1\times 2} & 0 \\ \hline 0 & 3|g|^2 + 2(\mu r)^2 \operatorname{Re}\left[\bar{g}\frac{g'}{\Xi^\varepsilon_-}\right] + (\mu r)^2\left|\frac{g'}{\Xi^\varepsilon_-}\right|^2 & \mathbf{0}_{1\times 2} & 0 \\ \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 1} & \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 1} \\ \hline 0 & 0 & \mathbf{0}_{1\times 2} & 0 \end{array}\right)$$

This concludes the proof. □

Having completed these preparatory computations of the momentum integrals appearing in Lemma 5.2.3, we can now further evaluate the expression for $\delta^2\mathcal{S}^\varepsilon$ for Lorentz boosts as given in (5.28b).

Lemma F.2.2 (Momentum Integration in Lemma 5.2.3)

By performing the momentum integrals, the expression for the second variation of the iε-regularized causal action for Lorentz boosts of the velocity vector of the regularization as derived in (5.28b) evaluates to

$$\begin{aligned} &\frac{1}{2\pi}\operatorname{Re}\left[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\left(\sqrt{\pi}Q_0^\varepsilon(|\vec{p}|) + \int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\;\frac{2\pi}{3}\,\frac{|\vec{p}||\vec{q}|Q_{10}^\varepsilon(|\vec{p}|,|\vec{q}|)}{\omega_p\omega_q}\right)\right] \\ &\quad = \int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0,r)\;\left(\xi^0 r^2 D\mathcal{L}^\varepsilon(\xi) + \frac{r^4}{3}D^2\mathcal{L}^\varepsilon(\xi)\right) - \int_{\mathbb{R}} \mathrm{d}\xi^0\;\frac{r^4}{3}\,\frac{\left(D\mathcal{L}^\varepsilon(\xi)\right)^2}{\partial_r\mathcal{L}^\varepsilon(\xi)}\bigg|_{r=R^\varepsilon_{\max}(\xi^0)} \end{aligned} \tag{F.7}$$

Proof. In order to prove the claimed equality, we compute the momentum integrals by invoking the results from Proposition F.2.1 and subsequently express the result in terms of combinations of the derivatives $D\mathcal{L}^\varepsilon(\xi)$ and $D^2\mathcal{L}^\varepsilon(\xi)$ of the regularized causal Lagrangian as computed in Appendix A.

(1) Evaluation of parts containing Q_0^ε

We start by evaluating those parts of the given expression which contain the function Q_0^ε. These are the first term as well as the δ-contribution implicitly contained in Q_{10}^ε in the second term.[a] By inserting the definition of Q_0^ε from (5.13a,i) we thus obtain

$$\begin{aligned} &\operatorname{Re}\left[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\;\sqrt{\pi}Q_0^\varepsilon(|\vec{p}|)\right] + \operatorname{Re}\left[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\;\frac{2\pi}{3}\,\frac{|\vec{p}||\vec{q}|Q_{10}^\varepsilon(|\vec{p}|,|\vec{q}|)}{\omega_p\omega_q}\right]^{\delta\text{-contr.}} \\ &\overset{\text{(5.13b,i)}}{=} \operatorname{Re}\left[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\;\sqrt{\pi}\left(1 - \frac{\varepsilon}{3}\frac{|\vec{p}|^2}{\omega_p}\right)Q_0^\varepsilon(|\vec{p}|)\right] \\ &\overset{\text{(5.13a,i)}}{=} -\frac{\varepsilon}{2\sqrt{\pi}}\operatorname{Re}\left[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}\;\left(1 - \frac{\varepsilon}{3}\frac{|\vec{p}|^2}{\omega_p}\right)\omega_p\Big\{\mathcal{F}\big[\mathcal{K}_{00}^\varepsilon\big](|\vec{p}|)\Big\}\right] \end{aligned}$$

Inserting the Hadamard product form of $\{\mathcal{F}\big[\mathcal{K}_{00}^\varepsilon\big](|\vec{p}|)\}$ as given in (F.1a) we arrive at

$$\ldots \overset{\text{(F.1a)}}{=} -\frac{\varepsilon}{4\pi}\operatorname{Re}\left[\int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0,r)\;\operatorname{tr}\left[r^2\mathfrak{C}_{\mathcal{K}}^\varepsilon\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^3}\left(\omega_p - \frac{\varepsilon}{3}|\vec{p}|^2\right)\mathrm{e}^{-\varepsilon\omega_p}E_{\mathcal{K}}^\varepsilon\big(\mathcal{Z}_{\mathcal{K}}\odot\mathfrak{K}_0^{\mathrm{T}}\big)\right]\right]$$

The momentum integrals appearing in this expression have already been evaluated in (F.5a) and (F.5b), respectively. Inserting these results along with the explicit form of the coefficient matrix $\mathcal{C}^\varepsilon_{\mathcal{K}}$ from (4.13a), computing the matrix product and finally taking the trace results in

$$\begin{aligned}\dots = -32\pi\,\mathrm{Re}\Bigg[&\varepsilon\mu\int\limits_{\mathcal{X}^\varepsilon}\mathrm{d}(\xi^0,r)\;\xi^0 r^2\Big[-\mathrm{i}\mu\frac{g'}{\Xi^\varepsilon_-}\Big(B^\varepsilon|\xi^\varepsilon|^2\bar{g}-C^\varepsilon(\xi^\varepsilon_-)^2 g\Big)\\&\qquad+\frac{\mathrm{i}}{\mu}g\Big(\big(B^\varepsilon\bar{g}-C^\varepsilon g\big)+\mathrm{i}\mu\big(B^\varepsilon\bar{h}+C^\varepsilon h\big)\Big)\Big]\\&+(\varepsilon\mu)^2\int\limits_{\mathcal{X}^\varepsilon}\mathrm{d}(\xi^0,r)\;r^2\Big[-\frac{g}{\mu^2}\big(B^\varepsilon\bar{g}+C^\varepsilon g\big)\Big]\\&+\frac{(\varepsilon\mu)^2}{3}\int\limits_{\mathcal{X}^\varepsilon}\mathrm{d}(\xi^0,r)\;r^4\Big[\frac{\mu^2}{(\Xi^\varepsilon_-)^2}\Big(g''-\frac{g'}{\Xi^\varepsilon_-}\Big)\Big(B^\varepsilon|\xi^\varepsilon|^2\bar{g}-C^\varepsilon(\xi^\varepsilon_-)^2 g\Big)\\&\qquad-\frac{g'}{\Xi^\varepsilon_-}\Big(2\big(B^\varepsilon\bar{g}-C^\varepsilon g\big)+\mathrm{i}\mu\big(B^\varepsilon\bar{h}+C^\varepsilon h\big)\Big)\Big]\Bigg]\end{aligned}$$

Comparing the integrand of the first term with the expression for $D\mathcal{L}^\varepsilon(\xi)$ as derived in (A.15a) we find that the result can be expressed in terms of $D\mathcal{L}^\varepsilon(\xi)$ such that we end up with the following intermediate result

$$\begin{aligned}\dots \overset{\text{(A.15a)}}{=} 2\pi&\int\limits_{\mathcal{X}^\varepsilon}\mathrm{d}(\xi^0,r)\;\xi^0 r^2 D\mathcal{L}^\varepsilon(\xi)\\&-32\pi\,\mathrm{Re}\Bigg[(\varepsilon\mu)^2\int\limits_{\mathcal{X}^\varepsilon}\mathrm{d}(\xi^0,r)\;r^2\Big[-\frac{g}{\mu^2}\big(B^\varepsilon\bar{g}+C^\varepsilon g\big)\Big]\\&\quad+\frac{(\varepsilon\mu)^2}{3}\int\limits_{\mathcal{X}^\varepsilon}\mathrm{d}(\xi^0,r)\;r^4\Big[\frac{\mu^2}{(\Xi^\varepsilon_-)^2}\Big(g''-\frac{g'}{\Xi^\varepsilon_-}\Big)\Big(B^\varepsilon|\xi^\varepsilon|^2\bar{g}-C^\varepsilon(\xi^\varepsilon_-)^2 g\Big)\\&\qquad-\frac{g'}{\Xi^\varepsilon_-}\Big(2\big(B^\varepsilon\bar{g}-C^\varepsilon g\big)+\mathrm{i}\mu\big(B^\varepsilon\bar{h}+C^\varepsilon h\big)\Big)\Big]\Bigg]\end{aligned}$$

(2) Evaluation of parts containing Q^ε_{10}

Having evaluated the parts which contain Q^ε_0, we now turn to the evaluation of the remaining parts of Q^ε_{10}, namely the bulk and boundary contributions.

(a) Bulk Contribution

We start by evaluating the bulk parts of the initial expression, i. e. those parts of Q^ε_{10} which contains the incomplete Fourier transforms $\{\mathcal{F}[\mathcal{M}^\varepsilon_{10|10}](|\vec{p}|,|\vec{q}|)\}$ and $\{\mathcal{F}[\mathcal{N}^\varepsilon_{10|10}](|\vec{p}|,|\vec{q}|)\}$. By inserting the definition of Q^ε_{10} from (5.13b,i) (without the already treated δ-contribution) we thus have

$$\begin{aligned}\mathrm{Re}&\left[\int\limits_0^\infty\frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\int\limits_0^\infty\frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\;\frac{2\pi}{3}\;\frac{|\vec{p}||\vec{q}|Q^\varepsilon_{10}(|\vec{p}|,|\vec{q}|)}{\omega_p\omega_q}\right]^{\text{bulk}} =\\&\overset{\text{(5.13b,i)}}{=}\mathrm{Re}\left[\frac{\varepsilon^2}{6\pi}\int\limits_0^\infty\frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^3}{(2\pi)^3}\,\mathrm{e}^{-\varepsilon\omega_p}\int\limits_0^\infty\frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^3}{(2\pi)^3}\,\mathrm{e}^{-\varepsilon\omega_q}\times\right.\\&\qquad\left.\times\Big(\Big\{\mathcal{F}\big[\mathcal{M}^\varepsilon_{10|10}\big](|\vec{p}|,|\vec{q}|)\Big\}+\Big\{\mathcal{F}\big[\mathcal{N}^\varepsilon_{10|10}\big](|\vec{p}|,|\vec{q}|)\Big\}\Big)\right]\end{aligned}$$

Inserting the Hadamard product form of $\{\mathcal{F}[\mathcal{M}^\varepsilon_{10|10}](|\vec{p}|,|\vec{q}|)\}$ and $\{\mathcal{F}[\mathcal{N}^\varepsilon_{10|10}](|\vec{p}|,|\vec{q}|)\}$ from (F.1b) and commuting asterisked terms to the end, we arrive at

$$\ldots \overset{\text{(F.1b)}}{=} \mathrm{Re}\Bigg[\frac{\varepsilon^2}{6\pi}\int\limits_{\mathcal{X}^\varepsilon} \mathrm{d}(\xi^0,r)\ \times \\ r^2\,\mathrm{tr}\Bigg[\mathcal{C}^\varepsilon_{\mathcal{M}}\int\limits_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^3}{(2\pi)^3}\,\mathrm{e}^{-\varepsilon\omega_p}\int\limits_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^3}{(2\pi)^3}\,\mathrm{e}^{-\varepsilon\omega_q}E^\varepsilon_{\mathcal{M}}\big(\mathcal{Z}\odot\mathfrak{M}^{\mathrm{T}}_{11}\big) \\ + \mathcal{C}^\varepsilon_{\mathcal{N}}\int\limits_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^3}{(2\pi)^3}\,\mathrm{e}^{-\varepsilon\omega_p}\int\limits_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^3}{(2\pi)^3}\,E^\varepsilon_{\mathcal{N}}\mathrm{e}^{-\varepsilon\omega_q}\big(\mathcal{Z}\odot\mathfrak{N}^{\mathrm{T}}_{11}\big) \\ + C^\varepsilon\mathbb{1}_5\int\limits_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^3}{(2\pi)^3}\,\mathrm{e}^{-\varepsilon\omega_p}\int\limits_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^3}{(2\pi)^3}\,E^\varepsilon_{\mathcal{M}}\mathrm{e}^{-\varepsilon\omega_q}\big(\mathcal{Z}\odot\overset{*}{\mathfrak{M}}{}^{\mathrm{T}}_{11}\big) \\ - B^\varepsilon\mathbb{1}_5\int\limits_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^3}{(2\pi)^3}\,\mathrm{e}^{-\varepsilon\omega_p}\int\limits_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^3}{(2\pi)^3}\,\mathrm{e}^{-\varepsilon\omega_q}E^\varepsilon_{\mathcal{N}}\big(\mathcal{Z}\odot\overset{*}{\mathfrak{N}}{}^{\mathrm{T}}_{11}\big)\Bigg]\Bigg]$$

The momentum integrals appearing in this expression have already been computed in (F.5c) - (F.5f). Inserting these results along with the explicit expressions for the coefficient matrices $\mathcal{C}^\varepsilon_{\mathcal{M}}$ and $\mathcal{C}^\varepsilon_{\mathcal{N}}$ from (4.19a,i) and (4.19b,i), respectively, carrying out the matrix multiplication, taking the trace and grouping terms according to their number and type of derivatives results in

$$\ldots \underset{\text{(F.5f)}}{\overset{\text{(F.5c)}}{=}} \mathrm{Re}\Bigg[\frac{32\pi}{3}(\varepsilon\mu)^2\int\limits_{\mathcal{X}^\varepsilon}\mathrm{d}(\xi^0,r)\ r^4\times \\ \Bigg[-\mu^2\Big(\frac{g'}{\Xi^\varepsilon_-}\Big)^2\Big(\big(|\xi^\varepsilon|^2\big)^2\bar{g}^2-(\xi^\varepsilon_-)^2C^\varepsilon\Big) \\ -\mu^2\Big|\frac{g'}{\Xi^\varepsilon_-}\Big|^2\Big(\big(|\xi^\varepsilon|^2\big)^2|g|^2-|\xi^\varepsilon|^2B^\varepsilon+4r^2|g|^2\,\mathrm{Re}\Big[|\xi^\varepsilon|^2-(\xi^\varepsilon_-)^2\Big]\Big) \\ +\frac{g'}{\Xi^\varepsilon_-}\Big(\mathrm{i}\mu\Big(2\bar{g}^2|\xi^\varepsilon|^2h+4|g|^2(\xi^\varepsilon_-)^2\bar{h}+2|g|^2|\xi^\varepsilon|^2\bar{h}\Big) \\ +4|g|^2\bar{g}(\xi^\varepsilon_-)^2-2\big(C^\varepsilon g+B^\varepsilon\bar{g}\big)\Big) \\ +\frac{1}{\mu^2}\Big(-2\big(|g|^2\big)^2-\mathrm{i}\mu|g|^2\Big(3g\bar{h}-\bar{g}h\Big)+\mu^2\big(|g|^2\big)^2\Big(|\xi^\varepsilon|^2+(\xi^\varepsilon_+)^2\Big)\Big) \\ -\frac{3}{(\mu r)^2}\big(C^\varepsilon g^2+B^\varepsilon|g|^2\big)\Bigg]\Bigg]$$

Comparing this expression with that of $D^2\mathcal{L}^\varepsilon(\xi)$ from (A.15b), we recognize a high degree of similarity though no equality. Expressing the above formula in terms of $D^2\mathcal{L}^\varepsilon(\xi)$ by adding and subtracting terms in a suitable way, we end up with

$$\ldots \overset{\text{(A.15b)}}{=} \frac{2\pi}{3}\int\limits_{\mathcal{X}^\varepsilon}\mathrm{d}(\xi^0,r)\ r^4D^2\mathcal{L}^\varepsilon(\xi)-\mathrm{Re}\Bigg[32\pi\varepsilon^2\int\limits_{\mathcal{X}^\varepsilon}\mathrm{d}(\xi^0,r)\ r^2\big(C^\varepsilon g^2+B^\varepsilon|g|^2\big)\Bigg] \\ +\mathrm{Re}\Bigg[\frac{32\pi}{3}(\varepsilon\mu)^2\int\limits_{\mathcal{X}^\varepsilon}\mathrm{d}(\xi^0,r)\ r^4\Bigg[\frac{\mu^2}{(\Xi^\varepsilon_-)^2}\Big(g''-\frac{g'}{\Xi^\varepsilon_-}\Big)\Big(B^\varepsilon|\xi^\varepsilon|^2\bar{g}-C^\varepsilon(\xi^\varepsilon_-)^2g\Big) \\ +\frac{g'}{\Xi^\varepsilon_-}\Big(2\big(C^\varepsilon g-B^\varepsilon\bar{g}\big)-\mathrm{i}\mu\big(B^\varepsilon\bar{h}+C^\varepsilon h\big)\Big)\Bigg]\Bigg]$$

(b) Boundary Contribution

Having computed the bulk contribution we now turn to the evaluation of the boundary terms, i. e. those parts of Q^ε_{10} which contains the incomplete Fourier transforms $\{\mathcal{F}[\mathcal{V}^\varepsilon_{10|10}](|\vec{p}|,|\vec{q}|)\}$ and $\{\mathcal{F}[\mathcal{W}^\varepsilon_{10|10}](|\vec{p}|,|\vec{q}|)\}$. By inserting the definition of Q^ε_{10} from (5.13b,i) (without the already treated δ-contribution and the bulk contribution) we thus have

$$\operatorname{Re}\left[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\;\frac{2\pi}{3}\,\frac{|\vec{p}||\vec{q}|Q^\varepsilon_{10}(|\vec{p}|,|\vec{q}|)}{\omega_p\omega_q}\right]^{\text{bndry}} =$$
$$= -\operatorname{Re}\Bigg[\frac{\varepsilon^2}{6\pi}\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^3}{(2\pi)^3}\;\mathrm{e}^{-\varepsilon\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^3}{(2\pi)^3}\;\mathrm{e}^{-\varepsilon\omega_q}\times$$
$$\times\Big(\Big\{\mathcal{F}\big[\mathcal{V}^\varepsilon_{10|10}\big](|\vec{p}|,|\vec{q}|)\Big\}+\Big\{\mathcal{F}\big[\mathcal{W}^\varepsilon_{10|10}\big](|\vec{p}|,|\vec{q}|)\Big\}\Big)\Bigg]$$

Inserting the Hadamard product form of $\{\mathcal{F}[\mathcal{V}^\varepsilon_{10|10}](|\vec{p}|,|\vec{q}|)\}$ and $\{\mathcal{F}[\mathcal{W}^\varepsilon_{10|10}](|\vec{p}|,|\vec{q}|)\}$ from (F.1c) we arrive at

$$\cdots = -\operatorname{Re}\Bigg[\frac{\varepsilon^2}{6\pi}\int_{\mathbb{R}}\mathrm{d}\xi^0\;\operatorname{tr}\Bigg[r^2\mathfrak{C}^\varepsilon_{\mathcal{V}}\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^3}{(2\pi)^3}\;\mathrm{e}^{-\varepsilon\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^3}{(2\pi)^3}\;\mathrm{e}^{-\varepsilon\omega_q}E^\varepsilon_{\mathcal{V}}\big(\mathfrak{Z}\odot\mathfrak{M}^{\mathrm{T}}_{11}\big)$$
$$+r^2\mathfrak{C}^\varepsilon_{\mathcal{W}}\int_0^\infty \frac{\mathrm{d}|\vec{p}|}{(2\pi)^3}\;|\vec{p}|^3\mathrm{e}^{-\varepsilon\omega_p}\int_0^\infty \frac{\mathrm{d}|\vec{q}|}{(2\pi)^3}\;|\vec{q}|^3\mathrm{e}^{-\varepsilon\omega_q}E^\varepsilon_{\mathcal{W}}\big(\mathfrak{Z}\odot\mathfrak{N}^{\mathrm{T}}_{11}\big)\Bigg]\Bigg|_{r=R^\varepsilon_{\max}(\xi^0)}\Bigg]$$

The momentum integrals appearing in this expression have already been computed in (F.5c) and (F.5d). Inserting these results along with the explicit expressions for the coefficient matrices $\mathfrak{C}^\varepsilon_{\mathcal{V}}$ and $\mathfrak{C}^\varepsilon_{\mathcal{W}}$ from (4.24a,ii) and (4.24b,ii), respectively, carrying out the matrix multiplication, taking the trace and grouping terms according to their number and type of derivatives results in

$$\cdots = -\operatorname{Re}\Bigg[\frac{256\pi}{3}(\varepsilon\mu)^2\int_{\mathbb{R}}\mathrm{d}\xi^0\;\frac{r^4}{\partial_r\mathcal{L}^\varepsilon(\xi)}\Bigg[$$
$$-\bigg[\mu\Big(B^\varepsilon|\xi^\varepsilon|^2\bar{g}-C^\varepsilon(\xi^\varepsilon_-)^2g\Big)\frac{g'}{\Xi^\varepsilon_-}-\frac{1}{\mu}g\Big(\big(B^\varepsilon\bar{g}-C^\varepsilon g\big)+\mathrm{i}\mu\big(B^\varepsilon\bar{h}+C^\varepsilon h\big)\Big)\bigg]^2$$
$$+\bigg|\mu\Big(B^\varepsilon|\xi^\varepsilon|^2\bar{g}-C^\varepsilon(\xi^\varepsilon_-)^2g\Big)\frac{g'}{\Xi^\varepsilon_-}-\frac{1}{\mu}g\Big(\big(B^\varepsilon\bar{g}-C^\varepsilon g\big)+\mathrm{i}\mu\big(B^\varepsilon\bar{h}+C^\varepsilon h\big)\Big)\bigg|^2\Bigg]\Bigg]$$
$$\cdots = -\frac{2\pi}{3}\int_{\mathbb{R}}\mathrm{d}\xi^0\;\frac{r^4}{\partial_r\mathcal{L}^\varepsilon(\xi)}\Bigg[8(\varepsilon\mu)\operatorname{Re}\bigg[\mathrm{i}\mu\Big(B^\varepsilon|\xi^\varepsilon|^2\bar{g}-C^\varepsilon(\xi^\varepsilon_-)^2g\Big)\frac{g'}{\Xi^\varepsilon_-}$$
$$-\frac{\mathrm{i}}{\mu}g\Big(\big(B^\varepsilon\bar{g}-C^\varepsilon g\big)+\mathrm{i}\mu\big(B^\varepsilon\bar{h}+C^\varepsilon h\big)\Big)\bigg]\Bigg]^2$$

where in the last equality we exploited the relation $2\operatorname{Re}(\mathrm{i}x)^2=\operatorname{Re}(-x^2+|x|^2)$. Comparing this expression with $D\mathcal{L}^\varepsilon(\xi)$ from (A.15a) we find that the integrand is proportional to the square of $\big(D\mathcal{L}^\varepsilon(\xi)\big)$ such that we end up with

$$\operatorname{Re}\left[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\;\frac{2\pi}{3}\,\frac{|\vec{p}||\vec{q}|Q^\varepsilon_{10}(|\vec{p}|,|\vec{q}|)}{\omega_p\omega_q}\right]^{\text{bndry}} \overset{\text{(A.15a)}}{=} -2\pi\int_{\mathbb{R}}\mathrm{d}\xi^0\;\frac{r^4}{3}\,\frac{\big(D\mathcal{L}^\varepsilon(\xi)\big)^2}{\partial_r\mathcal{L}^\varepsilon(\xi)}\bigg|_{r=R^\varepsilon_{\max}(\xi^0)} \tag{F.8}$$

for the boundary term.

(3) Conclusion

Adding up all the contributions computed above, we end up with

$$
\begin{aligned}
&\mathrm{Re}\left[\int_0^\infty \frac{\mathrm{d}|\vec{p}|\,|\vec{p}|^2}{(2\pi)^4}\left(\sqrt{\pi}Q_0^\varepsilon(|\vec{p}|) + \int_0^\infty \frac{\mathrm{d}|\vec{q}|\,|\vec{q}|^2}{(2\pi)^4}\,\frac{2\pi}{3}\,\frac{|\vec{p}||\vec{q}|Q_{10}^\varepsilon(|\vec{p}|,|\vec{q}|)}{\omega_p\omega_q}\right)\right] \\
&= 2\pi\int_{\mathfrak{X}^\varepsilon} \mathrm{d}(\xi^0,r)\;\xi^0 r^2 D\mathcal{L}^\varepsilon(\xi) \\
&\quad - 32\pi\,\mathrm{Re}\Bigg[(\varepsilon\mu)^2\int_{\mathfrak{X}^\varepsilon}\mathrm{d}(\xi^0,r)\;r^2\left[-\frac{g}{\mu^2}\cancelto{(1)}{\left(B^\varepsilon\bar{g}+C^\varepsilon g\right)}\right] \\
&\qquad + \frac{(\varepsilon\mu)^2}{3}\int_{\mathfrak{X}^\varepsilon}\mathrm{d}(\xi^0,r)\;r^4\Bigg[\frac{\mu^2}{(\Xi_-^\varepsilon)^2}\cancelto{(2)}{\left(g''-\frac{g'}{\Xi_-^\varepsilon}\right)}\left(B^\varepsilon|\xi^\varepsilon|^2\bar{g}-C^\varepsilon(\xi_-^\varepsilon)^2 g\right) \\
&\qquad\qquad - \cancelto{(3)}{\frac{g'}{\Xi_-^\varepsilon}}\left(2\left(B^\varepsilon\bar{g}-C^\varepsilon g\right)+\mathrm{i}\mu\left(B^\varepsilon\bar{h}+C^\varepsilon h\right)\right)\Bigg]\Bigg] \\
&\quad + \frac{2\pi}{3}\int_{\mathfrak{X}^\varepsilon}\mathrm{d}(\xi^0,r)\;r^4 D^2\mathcal{L}^\varepsilon(\xi) - 32\pi\,\mathrm{Re}\left[\varepsilon^2\int_{\mathfrak{X}^\varepsilon}\mathrm{d}(\xi^0,r)\;r^2\cancelto{\text{cancels (1)}}{\left(C^\varepsilon g^2+B^\varepsilon|g|^2\right)}\right] \\
&\quad + 32\pi\,\mathrm{Re}\Bigg[\frac{(\varepsilon\mu)^2}{3}\int_{\mathfrak{X}^\varepsilon}\mathrm{d}(\xi^0,r)\;r^4\Bigg[\frac{\mu^2}{(\Xi_-^\varepsilon)^2}\cancelto{\text{cancels (2)}}{\left(g''-\frac{g'}{\Xi_-^\varepsilon}\right)}\left(B^\varepsilon|\xi^\varepsilon|^2\bar{g}-C^\varepsilon(\xi_-^\varepsilon)^2 g\right) \\
&\qquad\qquad + \cancelto{\text{cancels (3)}}{\frac{g'}{\Xi_-^\varepsilon}}\left(2\left(C^\varepsilon g-B^\varepsilon\bar{g}\right)-\mathrm{i}\mu\left(B^\varepsilon\bar{h}+C^\varepsilon h\right)\right)\Bigg]\Bigg] \\
&\quad - 2\pi\int_{\mathbb{R}}\mathrm{d}\xi^0\,\frac{r^4}{3}\,\frac{\left(D\mathcal{L}^\varepsilon(\xi)\right)^2}{\partial_r\mathcal{L}^\varepsilon(\xi)}\Bigg|_{r=R_{\max}^\varepsilon(\xi^0)} \\
&= 2\pi\int_{\mathfrak{X}^\varepsilon}\mathrm{d}(\xi^0,r)\;\left(\xi^0 r^2 D\mathcal{L}^\varepsilon(\xi)+\frac{r^4}{3}D^2\mathcal{L}^\varepsilon(\xi)\right) - 2\pi\int_{\mathbb{R}}\mathrm{d}\xi^0\,\frac{r^4}{3}\,\frac{\left(D\mathcal{L}^\varepsilon(\xi)\right)^2}{\partial_r\mathcal{L}^\varepsilon(\xi)}\Bigg|_{r=R_{\max}^\varepsilon(\xi^0)} \qquad \text{(F.9)}
\end{aligned}
$$

This concludes the proof. □

[a] See the expression for Q_{lm}^ε as given in (5.13b,i).

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