

THE FERMIONIC ENTANGLEMENT
ENTROPY OF SPATIAL REGIONS IN
SCHWARZSCHILD AND MINKOWSKI
SPACETIME



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Preliminary Note

Parts of this thesis have already been published in the works [13] and [15] (sometimes in a slightly modified version) and are mostly joint work with the respective co-authors.

Similarly, some parts of this thesis will likely soon be published in the work [14] (sometimes in a slightly modified version) and are mostly joint work with the respective co-authors. Here the references are with respect to the unpublished version of January 29, 2024.

Abstract

In this thesis we define and study the fermionic entanglement entropy for spatial subregions in Schwarzschild and Minkowski spacetime. Our starting point is always the Dirac propagator corresponding to the vacuum state (for an observer at infinity). We then introduce an ultraviolet regularization and rewrite the respective propagator as pseudo-differential operator.

In Schwarzschild spacetime we consider the entanglement entropy of a black hole horizon. We use separation of variables, an integral representation of the propagator and methods from pseudo-differential operator calculus to explicitly compute the entanglement entropy of the horizon in the limiting case that the regularization tends to zero. It turns out that it equals a numerical constant times the number of angular momentum modes occupied at the horizon. A similar result is proven to hold for the Rényi entanglement entropies with Rényi index $\varkappa > \frac{2}{3}$.

In the case of Minkowski spacetime we study the entanglement entropy of bounded spatial subregions. We consider two limiting cases: one where the regularization goes to zero and one where the regularization is fixed and the size of the region tends to infinity. The corresponding limiting coefficient is obtained by applying a more general result from [15]. We then show the positivity of this coefficient and prove that it is proportional to the area of the considered region, giving an area law. The positivity is also proven to hold for the Rényi entanglement entropies with Rényi index $0 < \varkappa < 2$, the other main results in this part even apply for arbitrary Rényi entanglement entropies (with $\varkappa > 0$).

Zusammenfassung

Wir definieren und untersuchen die fermionische Verschränkungsentropie für räumliche Teilmengen in Schwarzschild- und Minkowski-Raumzeit. Unser Ausgangspunkt ist in jedem Fall der Dirac Propagator für den Vakuumzustand (aus der Sicht eines Beobachters im Unendlichen). Wir führen dann eine ultraviolett-Regularisierung ein und drücken den Propagator als Pseudodifferentialoperator aus.

In der Schwarzschild-Raumzeit betrachten wir die Verschränkungsentropie des Horizonts des schwarzen Lochs. Wir verwenden Trennung der Variablen, eine Integraldarstellung des Propagators und Methoden aus der Theorie der Pseudodifferentialoperatoren um die Verschränkungsentropie des Horizonts in dem Grenzfall, dass die Regularisierung gegen Null strebt, explizit zu berechnen. Es stellt sich heraus,

dass diese bis auf eine numerische Konstante proportional zur Anzahl der besetzten Winkelmoden am Horizont ist. Ein ähnliches Resultat ergibt sich für die Rényi Verschränkungsentropien mit Rényi Index $\varkappa > 2/3$.

Im Fall der Minkowski-Raumzeit beschäftigen wir uns mit der Verschränkungsentropie von beschränkten räumlichen Teilmengen. Wir betrachten zwei verschiedene Grenzfälle: Im einen lassen wir die Regularisierung gegen null gehen, im anderen fixieren wir die Regularisierung und lassen die Größe der betrachteten Region gegen unendlich streben. Wir erhalten einen Ausdruck für die führende Ordnung durch ein allgemeineres Resultat aus [15]. Wir zeigen dann, dass dieser Ausdruck positiv ist und proportional zur Oberfläche der betrachteten Region skaliert, was zu einem Oberflächengesetz führt. Die Positivität wird außerdem für die Rényi Verschränkungsentropien mit Rényi Index $\varkappa < 2$ bewiesen. Die anderen Hauptresultate in diesem Teil können sogar auf alle Rényi Verschränkungsentropien (mit $\varkappa > 0$) angewendet werden.

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1. Introduction

This chapter is based on [13, Section 1 and 2.3.1 and Notation 6.1] and [15, Sections 1 and 2.1] (partly with similar or same phrasing).

Entropy is often said to be a measure of the disorder of a physical system. However, there are various different notions of entropy and while the connection to disorder might still be evident for the entropy in classical statistical mechanics as introduced by Boltzmann and Gibbs, it is not so clear anymore for more abstract definitions of entropy like the Shannon and Rényi entropies in information theory or the von Neumann entropy for quantum systems. A more general way to phrase it would be that entropy measures the lack of knowledge or information about a physical system.

In this thesis our main objective is the so called *entanglement entropy*, which tells about non-classical correlations between subsystems of a composite quantum system [1, 26]. Moreover, our methods also apply to some cases of Rényi entanglement entropies. One reason, entanglement entropy is an interesting topic of current research is the discovery of the so-called *black hole information paradox* [23]. In this paradox a black hole and its outside is considered as composite quantum system, which in total is in a so called *pure state*. For such a state, the von Neumann entropies of the inside and outside coincide and the entanglement entropy of the composite system equals this quantity. This holds at all times due to the principle of unitary time evolution, which ensures that the overall state always stays pure. Now there are two main discoveries that lead to the paradox. One was Bekenstein's and Hawking's finding that black holes behave thermally if one interprets surface gravity as temperature and the area of the event horizon as entropy [3, 22]. The other one was the discovery of Hawking radiation and the resulting "evaporation" of a black hole [20, 21]. This evaporation leads to the decrease of the black hole itself and an increase of Hawking radiation over time. This implies that over time the Bekenstein-Hawking entropy of the inside of the black hole decreases and the von Neumann entropy of the outside increases. However, this leads to a contradiction of the above mentioned principle for the entanglement entropy of a pure state, if one identifies the Bekenstein-Hawking entropy of the inside with its von Neumann entropy. This paradox inspired the holographic principle [43, 45] and the current program of attempting to understand the structure of spacetime via information theory, entanglement entropy and gauge/gravity dualities [36, 25]. A crucial point in the paradox is the question whether the von Neumann entropy of the inside of a black hole really is proportional to its area. The largest part of this thesis (Chapter 4) is dedicated to this problem.

The idea that the entropy of a black hole scales like its area gave rise to the question if a so called *area law* holds for the entropy of other physical systems as well. This can be understood with the following thought experiment as described in [19, Section 6.1] with reference to [44]: Consider a system with mass M contained in a ball with radius R , which is not a black hole. Therefore, its mass M must be smaller than the mass of

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a black hole with radius R . Now let a spherical shell with this mass difference collapse onto the original system, leading to the formation of a black hole with radius R . Thus the Bekenstein-Hawking entropy of the resulting system is proportional to R^2 . Then, employing classical thermodynamical principles like the positivity and additivity of entropy together with the second law of thermodynamics (stating that entropy can only increase), it follows that the thermodynamical entropy of the original system must be smaller or equal to the resulting one, i.e. bounded by a constant times R^2 . This leads us to the question, if such an area bound or even an area law holds for the von Neumann entropy of the original system as well. Chapter 5 is dedicated to this problem in Minkowski spacetime.

As previously mentioned, this thesis is concerned with entanglement entropy. We here consider the *fermionic* case, where the many-particle system is composed of fermions satisfying the (Pauli-)Fermi-Dirac statistics. Moreover, for simplicity we consider the *quasi-free* case where the particles do not interact with each other. This makes it possible to express the entanglement entropy in terms of the reduced one-particle density operator [24] (for details see Section 2.1.2). This setting has been studied extensively for a free Fermi gas formed of non-relativistic spinless particles [24, 31, 32] (for more details see the preliminaries in Section 2.1.2). In the present thesis, we turn attention to a *relativistic* system formed of particles *with spin*.

The first main part (Chapter 4) of this thesis is based on the work [13]. It is devoted to the mathematical analysis of the entropy of the horizon of a Schwarzschild black hole with mass M . More precisely, we compute the entanglement entropy of the quasi-free fermionic Hadamard state which is obtained by frequency splitting for the observer in a rest frame at infinity, with an ultraviolet regularization on a length scale ε . We find that, up to a prefactor which depends on εM , this entanglement entropy is given by the number of occupied angular momentum modes, making it possible to reduce the computation of the entanglement entropy to counting the number of occupied states. A similar result is obtained for the Rényi entanglement entropies with Rényi index $\varkappa > \frac{2}{3}$. We choose the one-particle density operator as the regularized projection operator to all negative-frequency solutions of the Dirac equation in the exterior Schwarzschild geometry (where frequency splitting refers to the Schwarzschild time of an observer at rest at infinity). Making use of the integral representation of the Dirac propagator in [11] and employing techniques developed in [31, 49, 40, 41, 39], it becomes possible to compute the entanglement entropy of the black hole horizon explicitly.

More precisely, the general definition of the Rényi entanglement entropy is given as follows. First of all, we denote by $\Pi^{(\varepsilon)}$ the regularized projector to the negative frequency solutions of the Dirac equation in a given spacetime (in our cases this will either be Schwarzschild or Minkowski spacetime). Moreover, for each $\varkappa > 0$ we introduce the *Rényi entropy function*, which is defined as follows. If $t \notin [0, 1]$ then we set $\eta_\varkappa(t) := 0$. For $t \in [0, 1]$ we define

$$\begin{aligned} \eta_\varkappa(t) &:= \frac{1}{1-\varkappa} \ln(t^\varkappa + (1-t)^\varkappa) && \text{for } \varkappa \neq 1, \\ \eta(t) &:= \eta_1(t) := \lim_{\varkappa \rightarrow 1} \eta_\varkappa(t) = -t \ln t - (1-t) \ln(1-t) && \text{for } \varkappa = 1, \end{aligned} \tag{1.1}$$

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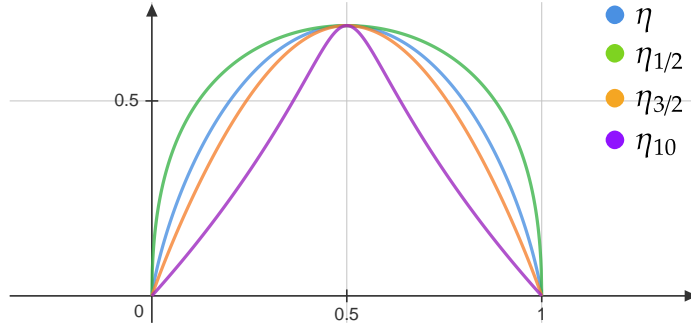


Figure 1.1.: Plot of the Rényi entropy functions η , $\eta_{1/2}$, $\eta_{3/2}$ and η_{10} for $t \in [0, 1]$. Note that all displayed functions are non-negative and vanish at $t = 0$ and $t = 1$. Further, η , $\eta_{1/2}$ and $\eta_{3/2}$ are concave. Moreover, the derivatives of η and $\eta_{1/2}$ tend to infinity for $t \searrow 0$ and $t \nearrow 1$.

(for a plot see 1.1). Where $\eta \equiv \eta_1$ describes the von Neumann entropy of the corresponding fock state. Therefore the case $\varkappa = 1$ describes the ordinary entanglement entropy, which we are mainly interested in. Similarly, the functions η_\varkappa describe the Rényi entropies of the corresponding fock state (a detailed derivation of both these cases can be found in [14, Appendix A]). Now, for any spatial subset $\Lambda \subset \mathbb{R}^d$ (always assumed non-empty) we can define the *Rényi entanglement entropy* associated with the bi-partition $\Lambda \cup \Lambda^c$ (see e.g. [30, Section 3]):

$$S_\varkappa(\Pi^{(\varepsilon)}, \Lambda) := \text{tr} \left(\eta_\varkappa(\chi_\Lambda \Pi^{(\varepsilon)} \chi_\Lambda) - \chi_\Lambda \eta_\varkappa(\Pi^{(\varepsilon)}) \chi_\Lambda \right). \quad (1.2)$$

In the Schwarzschild case we denote the regularized projection operator to the negative frequency solutions of the Dirac equation by $\Pi_{\text{BH}}^{(\varepsilon)}$. In order to obtain the entropy of the horizon, we choose Λ as an annular region around the horizon of width ρ and denote it by $\tilde{\mathcal{K}}$, i.e. using the Regge-Wheeler coordinate $u \in \mathbb{R}$,

$$\begin{aligned} \tilde{\mathcal{K}} &:= (u_0 - \rho, u_0) \times S^2 \\ &\equiv \left\{ \begin{pmatrix} u \sin \vartheta \cos \phi \\ u \sin \vartheta \sin \phi \\ u \cos \vartheta \end{pmatrix} \middle| u_0 - \rho < u < u_0, \ 0 < \vartheta < \pi, \ 0 < \phi < 2\pi \right\} \end{aligned} \quad (1.3)$$

(see also Figure 4.1 on page 43). In these coordinates, the horizon is located at $u \rightarrow -\infty$. Therefore, the Rényi entanglement entropy is given by $S_\varkappa(\Pi_{\text{BH}}^{(\varepsilon)}, \tilde{\mathcal{K}})$ in the limit $u_0 \rightarrow -\infty$. We shall prove that, to leading order in the regularization length ε , this trace is independent of ρ . It turns out that we get equal contributions from the two boundaries at $u_0 - \rho$ and u_0 as $u_0 \rightarrow -\infty$. Therefore, the fermionic entanglement entropy is given by one half this trace.

Before stating our main result, we note that the trace of the entropic difference operator can be decomposed into a sum over all occupied angular momentum modes (we will make this precise in Section 4.2.1), i.e.

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$$\begin{aligned}
S_{\varkappa}(\Pi_{\text{BH}}^{(\varepsilon)}, \tilde{\mathcal{K}}) &= \sum_{\substack{(k,n) \\ \text{occupied}}} \text{tr} \left(\eta_{\varkappa}(\chi_{\mathcal{K}} \text{Op}_{\alpha}((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}) \chi_{\mathcal{K}}) - \chi_{\mathcal{K}} \eta_{\varkappa}(\text{Op}_{\alpha}((\Pi_{\text{BH}}^{(\varepsilon)})_{kn})) \chi_{\mathcal{K}} \right) \\
&= \sum_{\substack{(k,n) \\ \text{occupied}}} S_{\varkappa}((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}, \mathcal{K}),
\end{aligned}$$

where $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$ can be thought of as diagonal block element of $\Pi_{\text{BH}}^{(\varepsilon)}$ acting on a subspace of the solution space corresponding to the given angular mode. As a consequence of the mode decomposition, the characteristic function $\chi_{\tilde{\mathcal{K}}}$ goes over to $\chi_{\mathcal{K}}$ with

$$\mathcal{K} := (u_0 - \rho, u_0). \quad (1.4)$$

We define the *mode-wise Rényi entanglement entropy* of the black hole as

$$S_{\varkappa, kn}^{\text{BH}} := \frac{1}{2} \lim_{\rho \rightarrow \infty} \lim_{\varepsilon \searrow 0} \frac{1}{f(\varepsilon)} \lim_{u_0 \rightarrow -\infty} S_{\varkappa}((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}, \mathcal{K}), \quad (1.5)$$

where $f(\varepsilon)$ is a function describing the highest order of divergence in ε (we will later see that here $f(\varepsilon) = \ln(M/\varepsilon)$ where M is the black hole mass). Finally, the resulting *fermionic Rényi entanglement entropy operator* of the black hole can be written as the sum of the entropies of all occupied modes,

$$S_{\varkappa}^{\text{BH}} = \sum_{\substack{(k,n) \\ \text{occupied}}} S_{\varkappa, kn}^{\text{BH}}. \quad (1.6)$$

Our main result shows that $S_{\varkappa, kn}^{\text{BH}}$ has the same numerical value for each angular mode.

Theorem 1.0.1. *Let $\varkappa > \frac{2}{3}$, $n \in \mathbb{Z}$ and $k \in \mathbb{Z} + 1/2$ arbitrary, then*

$$\lim_{\varepsilon \searrow 0} \lim_{u_0 \rightarrow -\infty} \frac{1}{\ln(M/\varepsilon)} S_{\varkappa}((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}, \mathcal{K}) = \frac{1}{2\pi^2} U(1; \eta_{\varkappa}) = \frac{1}{12} \frac{\varkappa + 1}{\varkappa},$$

where M is the black hole mass.

In simple terms, this result shows that each occupied angular momentum mode gives the same contribution to the Rényi entanglement entropy. This makes it possible to compute the entanglement entropy of the horizon simply by counting the number of occupied angular momentum modes. This is reminiscent of the counting of states in string theory [42] and loop quantum gravity [2]. In order to push the analogy further, assuming a minimal area ε^2 on the horizon, the number of occupied angular modes should scale like M^2/ε^2 . In this way, we find that the entanglement entropy is indeed proportional to the area of the black hole. More precisely, the factor $\ln(M/\varepsilon)$ in the above theorem can be understood as an enhanced area law. We point out that, in our case, the counting takes place in the four-dimensional Schwarzschild geometry.

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In the second main part (Chapter 5), which is based on the work [15], we consider a free Dirac field in a bounded spatial subset of Minkowski spacetime. We compute the entanglement entropy for the quantum state describing the vacuum with an ultraviolet regularization on a length scale ε . The corresponding one-particle density operator turns out to be the regularized projection operator to all negative-frequency solutions of the Dirac equation. Making use of the explicit form of the Dirac propagator and employing the techniques developed in [15], it becomes possible to compute the limiting coefficient of the entanglement entropy of bounded spatial subregions in Minkowski spacetime. Using the Lorentz invariance of the Dirac equation and the concavity of the Rényi entropy functions we prove an area law in two limiting cases: that the volume tends to infinity and that the regularization goes to zero.

More precisely, let $\Pi_{\text{MI}}^{(\varepsilon)}$ be the projection onto the negative frequency subspace of the Dirac operator in Minkowski spacetime. Our main objective is to analyze the asymptotic behavior of the entropy $S_{\varkappa}(\Pi_{\text{MI}}^{(\varepsilon)}, L\Lambda)$ as the regularization parameter ε tends to zero and/or the *scaling parameter* L tends to infinity.

The following theorem constitutes the main result of this chapter – it provides the area law for the asymptotics of the entanglement entropy.

Theorem 1.0.2. *Let $\Lambda \subset \mathbb{R}^3$ be a bounded open spatial region of Minkowski spacetime with C^1 -boundary consisting of finitely many connected components. Then, as $L\varepsilon^{-1} \rightarrow \infty$ and $\varepsilon \rightarrow 0$, the following asymptotics hold:*

$$\lim L^{-2}\varepsilon^2 S_{\varkappa}(\Pi_{\text{MI}}^{(\varepsilon)}, L\Lambda) = \mathfrak{M}_{\varkappa} \text{vol}_2(\partial\Lambda), \quad (1.7)$$

where \mathfrak{M}_{\varkappa} is some explicit constant.

If $L \rightarrow \infty$ and $\varepsilon > 0$ is fixed, then

$$\lim L^{-2}\varepsilon^2 S_{\varkappa}(\Pi_{\text{MI}}^{(\varepsilon)}, L\Lambda) = \mathfrak{M}_{\varkappa}^{(\varepsilon)} \text{vol}_2(\partial\Lambda), \quad (1.8)$$

where $\mathfrak{M}_{\varkappa}^{(\varepsilon)}$ is some explicit constant such that $\mathfrak{M}_{\varkappa}^{(\varepsilon)} \rightarrow \mathfrak{M}_{\varkappa}$ as $\varepsilon \rightarrow 0$.

If $0 < \varkappa < 2$, then both coefficients \mathfrak{M}_{\varkappa} and $\mathfrak{M}_{\varkappa}^{(\varepsilon)}$ are strictly positive.

The definitions of the coefficients \mathfrak{M}_{\varkappa} and $\mathfrak{M}_{\varkappa}^{(\varepsilon)}$ require more technical preliminaries and are given in Section 5.5.

The technical core of the results in this thesis relies on rewriting the regularized projector in each spacetime as pseudo-differential operator of the form

$$\left(\text{Op}_{\alpha}(\mathcal{A})\psi\right)(\mathbf{x}) := \left(\frac{\alpha}{2\pi}\right)^d \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} e^{-i\alpha\xi \cdot (\mathbf{x}-\mathbf{y})} \mathcal{A}(\mathbf{x}, \mathbf{y}, \xi) \psi(\mathbf{y}) \, d\mathbf{y} \, d\xi,$$

for suitable functions ψ from \mathbb{R}^d to \mathbb{C}^n . The parameter $\alpha \in \mathbb{R}$ will play the role of the limiting parameter (e.g. ε^{-1} or $L\varepsilon^{-1}$). The matrix-valued function $\mathcal{A} \in L^1_{\text{loc}}(\mathbb{R}^{3d}, \mathbb{C}^{n \times n})$ is referred to as the *symbol* of the pseudo-differential operator (for more details on this see Section 2.2.1). In the case that $\text{Op}_{\alpha}(\mathcal{A})$ defines a self-adjoint operator on $L^2(\mathbb{R}^d, \mathbb{C}^n)$, we define for measurable functions f and subregions $\Lambda \subseteq \mathbb{R}^d$ the operator

$$D_{\alpha}(f, \Lambda, \mathcal{A}) := f(\chi_{\Lambda} \text{Op}_{\alpha}(\mathcal{A}) \chi_{\Lambda}) - \chi_{\Lambda} f(\text{Op}_{\alpha}(\mathcal{A})) \chi_{\Lambda}. \quad (1.9)$$

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When rewriting $\Pi^{(\varepsilon)}$ as pseudo-differential operator, its symbol usually depends on the regularization length ε . We denote this by a super- or subscript ε , e.g.

$$\Pi^{(\varepsilon)} = \text{Op}_\alpha(\mathcal{A}^{(\varepsilon)}),$$

for a suitable symbol $\mathcal{A}^{(\varepsilon)}$ and suitable a choice of α . Then, we may also rewrite the Rényi entanglement entropy as

$$S_\varkappa(\Pi^{(\varepsilon)}, \Lambda) = \text{tr} D_\alpha(\eta_\varkappa, \Lambda, \mathcal{A}^{(\varepsilon)}).$$

We are then usually interested in the limit where $\varepsilon \searrow 0$ and $\alpha \rightarrow \infty$ at the same time (except for the result (1.8)). There are some previously established results, which give more explicit formulas for (1.9) in the limit $\alpha \rightarrow \infty$, but often only for symbols that do not depend on ε (or α) and/or only for functions f which are more regular than the Rényi entropy functions (for example in [49] or [47]).

Therefore, in Chapter 4 the idea is to generalize one of these results and apply it to a simplified limiting symbol which is related to the limit of the symbol $\mathcal{A}^{(\varepsilon)}$ as $\varepsilon \searrow 0$ and does not depend on ε anymore. The error caused by replacing the symbol in such a way then needs to be estimated. To this end we employ several different techniques and previously established estimates mostly from the theory of pseudo-differential operator calculus.

In Chapter 5 (i.e. the Minkowski case) the procedure presented in this thesis is a little different. This is because we take the limiting coefficient (which is established in [15] with methods related to the ones just described) as given and focus on proving that it is positive and proportional to the area of the considered region, resulting in the area law. As we will see, the proportionality to the area can be derived using the symmetry of the Dirac equation. The positivity follows using a well-known result going back to Berezin from [4] together with the fact that the Rényi entropy functions η_\varkappa are strictly concave for $0 < \varkappa < 2$.

The thesis is structured as follows. We start with some general preliminaries in Chapter 2. The physical preliminaries (Section 2.1) contain general information on the Dirac equation (Section 2.1.1) and on the entanglement entropy of a fermionic quantum fock state (Section 2.1.2). The second part of this chapter (Section 2.2) is concerned with some technical preliminaries such as the precise definition of $\text{Op}_\alpha(\mathcal{A})$ and some useful norms (Section 2.2.1). Moreover, we collect some previously established estimates mainly on pseudo-differential operators (Section 2.2.2 and Section 2.2.3), which we will need among others to generalize a result for (1.9) in the limit $\alpha \rightarrow \infty$ as well as estimate the error terms.

Some more helpful tools for working with pseudo-differential operators are established in Section 3.

Chapter 4 is dedicated to the analysis of the entanglement entropy of a Schwarzschild black hole. The chapter begins by providing necessary preliminaries on the Schwarzschild Propagator in Section 4.1. Then (Section 4.2), the regularized projection operator to the negative-frequency solutions of the Dirac equation is defined and decomposed into angular momentum modes. For each angular momentum mode, the resulting functional calculus is formulated and the corresponding operator is rewritten

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in the language of pseudo-differential operators. Moreover, the symbol will be further simplified at the horizon. After these preparations, we can give a mathematical definition of the entanglement entropy of the black hole (Section 4.3). Following the preparations, the core of the work begins in Section 4.4, where we calculate the entropy corresponding to a simplified limiting operator (in the sense that the regularization goes to zero) at the horizon by generalizing a theorem by Widom (Theorem 4.4.2). Afterwards (Section 4.5) we estimate the error caused by using the limiting operator instead of the regularized one. It turns out that it drops out in the limiting process. Subsequently (Section 4.6) we complete the proof of the main result (Theorem 1.0.1) by combining the results from the previous sections.

In Chapter 5 we analyze the entanglement entropy of bounded spatial regions in Minkowski spacetime. Again we start our analysis by recalling a few physical preliminaries on the Dirac equation in Minkowski spacetime (Section 5.1). In Section 5.2 we provide some mathematical background of our analysis including an asymptotic formula by H. Widom, see Proposition 5.2.2. Moreover we state two results from [15] giving a formula for the limiting coefficient. Using these results we prove an abstract area law in Section 5.3. In Section 5.4 we use a well-known result going back to Berezin from [4] for concave functions to examine the positivity of the asymptotic coefficient. Afterwards, in Section 5.5 the results of Sections 5.2 and 5.4 are applied to the entanglement entropy $S_{\mathcal{Z}}(\Pi^{(\varepsilon)}, L\Lambda)$ to complete the proof of our main result, Theorem 1.0.2.

We finally discuss conclusions and open problems (Section 6).

Moreover, note that some detailed computations and proofs have been moved to the appendices A, B and C.

Units and notational conventions.

- We work throughout in natural units $\hbar = c = 1$. Then the only remaining unit is that of a length (measured for examples in meters). It is most convenient to work with dimensionless quantities. This can be achieved by choosing an arbitrary reference length ℓ and multiplying all dimensional quantities by suitable powers of ℓ . For example, we work with the

$$\text{dimensionless quantities} \quad m\ell, \quad \omega\ell, \quad \xi\ell, \quad \mathbf{k}\ell, \quad \frac{\mathbf{x}}{\ell}, \quad \frac{u}{\ell}, \quad \frac{\varepsilon}{\ell} \quad \text{etc..} \quad (1.10)$$

For ease in notation, in what follows we set $\ell = 1$, making it possible to leave out all powers of ℓ . The dimensionality can be recovered by rewriting all formulas using the dimensionless quantities in (1.10).

In the Schwarzschild case we will think of ℓ as the black hole mass M .

- For two non-negative numbers (or functions) X and Y depending on some parameters, we write $X \lesssim Y$ (or $Y \gtrsim X$) if $X \leq CY$ for some positive constant C independent of those parameters. To avoid confusion we may comment on the nature of (implicit) constants in the bounds. If $X \lesssim Y \lesssim X$, we write $X \simeq Y$.

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- By \mathcal{F} we denote the unitary extension of the Fourier transform to $L^2(\mathbb{C}^d, \mathbb{R}^n)$, which for any $\psi \in L^1(\mathbb{C}^d, \mathbb{R}^n)$ is given by

$$(\mathcal{F}\psi)(\boldsymbol{\xi}) := \frac{1}{\sqrt{(2\pi)^d}} \int e^{-i\boldsymbol{\xi}\mathbf{x}} \psi(\mathbf{x}) d\mathbf{x}.$$

- In the following we can sometimes factor out a characteristic function in $\boldsymbol{\xi}$ in the a symbol \mathcal{A} , i.e.

$$\mathcal{A}(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi}) = \chi_\Omega(\boldsymbol{\xi}) \tilde{\mathcal{A}}(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi}).$$

In this case, we will sometimes denote the characteristic function in $\boldsymbol{\xi}$ corresponding to the set Ω by I_Ω . This is to avoid confusion with the characteristic functions χ_Λ in the variables \mathbf{x} or \mathbf{y} .

- For any two bounded self-adjoint operators A and B on the Hilbert space \mathcal{H} the inequality $A \leq B$ is understood in the standard quadratic form sense:

$$(Au, u) \leq (Bu, u), \quad \text{for all } u \in \mathcal{H}.$$

- For any matrix \mathcal{B} the notation $|\mathcal{B}|$ stands for its Hilbert-Schmidt norm. In the case that $\mathcal{B} = \mathcal{B}(\boldsymbol{\xi})$, $\boldsymbol{\xi} \in \mathbb{R}^d$, is a smooth matrix-valued function then we write

$$|\nabla_{\boldsymbol{\xi}}^l \mathcal{B}(\boldsymbol{\xi})| = \sum_{|\mathbf{m}|=l} |\partial_{\boldsymbol{\xi}}^{\mathbf{m}} \mathcal{B}(\boldsymbol{\xi})|,$$

where $\partial_{\boldsymbol{\xi}}^{\mathbf{m}}$ is the standard partial derivative of order $\mathbf{m} \in \mathbb{Z}_+^d$.

- For operators on a normed space we denote the ordinary operator norm by $\|\cdot\|_\infty$.
- For n -component functions $\psi : \mathbb{R}^d \rightarrow \mathbb{R}^n$ the pointwise norm in \mathbb{C}^n will be denoted by $|\cdot|$, the canonical inner product on $L^2(\mathbb{R}^d, \mathbb{C}^n)$ by $\langle \cdot | \cdot \rangle$ and the corresponding norm by $\|\cdot\|$. In particular this holds for $d = 1$, $n = 2$ and the two-component functions of the form

$$A := \begin{pmatrix} A_+ \\ A_- \end{pmatrix},$$

which will come up in Chapter 4.

- For $\boldsymbol{\xi} \in \mathbb{R}^d$ we denote

$$\langle \boldsymbol{\xi} \rangle := \sqrt{1 + |\boldsymbol{\xi}|^2}.$$

- The symbol $\text{vol}_n(\Omega)$ with $n = 0, 1, \dots, d$ stands for the induced n -dimensional Lebesgue measure of the measurable set $\Omega \subset \mathbb{R}^d$.
- We call $\Omega \subset \mathbb{R}^d$ a *region* if it is a non-empty open set with finitely many connected components such that their closures are disjoint.
- The symbol $\mathbb{C}^{n \times k}$ denotes the space of all $(n \times k)$ -matrices.

1. Introduction

- Let $f : \mathbb{R}^d \rightarrow \mathbb{C}^{n \times k}$ be a function, then we denote the operator

$$\begin{aligned} \{\psi \mid \psi : \mathbb{R}^n \rightarrow \mathbb{C}^k\} &\rightarrow \{\psi \mid \psi : \mathbb{R}^n \rightarrow \mathbb{C}^n\}, \\ (\mathbf{x} \mapsto \psi(\mathbf{x})) &\mapsto (\mathbf{x} \mapsto f(\mathbf{x})\psi(\mathbf{x})), \end{aligned}$$

in some cases (for simplicity) again by f , or in other cases (for clarity) by \mathcal{M}_f .

- We denote the characteristic functions of the half-spaces \mathbb{R}^+ and \mathbb{R}^- by

$$\chi_+ := \chi_{\mathbb{R}^+}, \quad \chi_- := \chi_{\mathbb{R}^-}.$$

- For any vector space V we denote

$$L(V) := \{f : V \rightarrow V \mid f \text{ bounded and linear}\}.$$

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2.1. Physical Preliminaries

2.1.1. The Dirac Equation in Globally Hyperbolic Spacetimes

This section corresponds to [13, Section 2.2] (with slight modifications).

The abstract setting for the Dirac equation is given as follows (for more details see for example [16]). Our starting point is a four-dimensional, smooth, globally hyperbolic Lorentzian spin manifold (\mathcal{M}, g) , with metric g of signature $(+, -, -, -)$. We denote the corresponding spinor bundle by $S\mathcal{M}$. Its fibres $S_x\mathcal{M}$ are endowed with an inner product $\langle \cdot | \cdot \rangle_x$ of signature $(2, 2)$, referred to as the spin inner product. Moreover, the mapping

$$\gamma : T_x\mathcal{M} \rightarrow \mathbb{L}(S_x\mathcal{M}), \quad u \mapsto \sum_{j=0}^3 \gamma^j u_j,$$

where the γ^j are the Dirac matrices defined via the anti-commutation relations

$$\gamma(u) \gamma(v) + \gamma(v) \gamma(u) = 2 g(u, v) \mathbb{1}_{S_x(\mathcal{M})},$$

provides the structure of a Clifford multiplication.

Smooth sections in the spinor bundle are denoted by $C^\infty(\mathcal{M}, S\mathcal{M})$. Likewise, the space $C_0^\infty(\mathcal{M}, S\mathcal{M})$ are the smooth sections with compact support. We also refer to sections in the spinor bundle as *wave functions*. The Dirac operator \mathcal{D} takes the form

$$\mathcal{D} := i \sum_{j=0}^3 \gamma^j \nabla_j : C^\infty(\mathcal{M}, S\mathcal{M}) \rightarrow C^\infty(\mathcal{M}, S\mathcal{M}),$$

where ∇ denotes the connections on the tangent bundle and the spinor bundle. Then the Dirac equation with parameter m (in the physical context corresponding to the particle mass) reads

$$(\mathcal{D} - m) \psi = 0,$$

(for more details on the Dirac equation see [46] or [12, Sections 1.2-1.4 and 4.2-4.4]).

Due to global hyperbolicity, our spacetime admits a foliation by Cauchy surfaces $\mathcal{M} = (\mathcal{N}_t)_{t \in \mathbb{R}}$. Smooth initial data on any such Cauchy surface yield a unique global solution of the Dirac equation. Our main focus lies on smooth solutions with spatially compact support, denoted by $C_{sc}^\infty(\mathcal{M}, S\mathcal{M})$. The solutions in this class are endowed with the scalar product

$$(\psi | \phi) = \sum_{j=0}^3 \int_{\mathcal{N}} \langle \psi | \nu^j \gamma_j \phi \rangle_x d\mu_{\mathcal{N}}(x), \quad (2.1)$$

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where \mathcal{N} is a Cauchy surface with future-directed normal ν and $d\mu_{\mathcal{N}}$ denotes the measure on \mathcal{N} induced by the metric g (compared to the conventions in [16], we here preferred to leave out a factor of 2π). This scalar product is independent on the choice of \mathcal{N} (for details see [16, Section 2]). Finally we define the Hilbert space $(\mathcal{H}, \langle \cdot | \cdot \rangle)$ by completion,

$$\mathcal{H} := \overline{C_{sc}^{\infty}(\mathcal{M}, S\mathcal{M})}^{\langle \cdot | \cdot \rangle}. \quad (2.2)$$

2.1.2. The Entanglement Entropy of a Quasi-Free Fermionic Quantum State

The first part of this section corresponds to the first part of [15, Section 2.2] and the second part to [13, Remark 2.1] (both with slight modifications).

Given a Hilbert space $(\mathcal{H}, \langle \cdot | \cdot \rangle_{\mathcal{H}})$ (the ‘‘one-particle Hilbert space’’), we let $(\mathcal{F}, \langle \cdot | \cdot \rangle_{\mathcal{F}})$ be the corresponding fermionic Fock space, i.e.

$$\mathcal{F} = \bigoplus_{k=0}^{\infty} \underbrace{\mathcal{H} \wedge \cdots \wedge \mathcal{H}}_{k \text{ factors}}$$

(where \wedge denotes the totally anti-symmetrized tensor product). We define the *creation operator* Ψ^{\dagger} by

$$\Psi^{\dagger} : \mathcal{H} \rightarrow \mathcal{L}(\mathcal{F}), \quad \Psi^{\dagger}(\psi)(\psi_1 \wedge \cdots \wedge \psi_p) := \psi \wedge \psi_1 \wedge \cdots \wedge \psi_p.$$

Its adjoint is the *annihilation operator* denoted by $\Psi(\bar{\psi}) := (\Psi^{\dagger}(\psi))^*$. These operators satisfy the canonical anti-commutation relations

$$\{\Psi(\bar{\psi}), \Psi^{\dagger}(\phi)\} = (\psi | \phi) \quad \text{and} \quad \{\Psi(\bar{\psi}), \Psi(\bar{\phi})\} = 0 = \{\Psi^{\dagger}(\psi), \Psi^{\dagger}(\phi)\}.$$

Next, we let W be a *statistical operator* on \mathcal{F} , i.e. a positive semi-definite linear operator of trace one,

$$W : \mathcal{F} \rightarrow \mathcal{F}, \quad W \geq 0 \quad \text{and} \quad \text{tr}_{\mathcal{F}}(W) = 1.$$

Given an *observable* A (i.e. a symmetric operator on \mathcal{F}), the expectation value of the measurement is given by

$$\langle A \rangle := \text{tr}_{\mathcal{F}}(AW).$$

The corresponding *quantum state* ω is the linear functional which to every observable associates the expectation value, i.e.

$$\omega : A \mapsto \text{tr}_{\mathcal{F}}(AW).$$

The *von Neumann entropy* of the state ω is defined by

$$S_1(\omega) := -\text{tr}_{\mathcal{F}}(W \ln W).$$

In this thesis, we restrict our attention to the subclass of so-called *quasifree* states, fully determined by their two-point functions

$$\omega_2(\bar{\psi}, \phi) := \omega(\Psi(\bar{\psi}) \Psi^{\dagger}(\phi)), \quad \text{for any } \psi, \phi \in \mathcal{H}.$$

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Definition 2.1.1. *The reduced one-particle density operator D is the positive linear operator on the Hilbert space $(\mathcal{H}, \langle \cdot | \cdot \rangle_{\mathcal{H}})$ defined by*

$$\omega_2(\overline{\psi}, \phi) = \langle \psi | D\phi \rangle_{\mathcal{H}}, \quad \text{for any } \psi, \phi \in \mathcal{H}.$$

The von Neumann entropy $S_1(\omega)$ of the quasi-free fermionic quantum state can be expressed in terms of the reduced one-particle density operator by

$$S_1(\omega) = \text{tr } \eta(D), \tag{2.3}$$

where $\eta = \eta_1$ is the von Neumann entropy function defined in (1.1). This formula appears commonly in the literature (see for example [35, Equation 6.3], [27, 9, 33] and [24, eq. (34)]). A detailed derivation can be found in [14, Appendix A]. Similar to (2.3) also other entropies can be expressed in terms of the reduced one-particle density operator. Namely, the Rényi entropy and the corresponding entanglement entropy can be written as $S_{\kappa}(\omega) = \text{tr } \eta_{\kappa}(D)$ and (1.2), respectively. These formulas are also derived in [14, Appendix A].

We here consider a quasi-free state formed of solutions of the Dirac equation. Thus we choose the Hilbert space \mathcal{H} as the solution space of the Dirac equation with scalar product $\langle \cdot | \cdot \rangle_{\mathcal{H}} = \langle \cdot | \cdot \rangle$. Moreover, we consider the *regularized vacuum state*, in which case the reduced two-particle density operator is equal to the regularized projection operator onto all negative-frequency solutions of the Dirac equation in the respective spacetime, i.e.

$$D = \Pi^{(\varepsilon)}.$$

with $\Pi^{(\varepsilon)}$ as in (5.5). We point out that, in the limiting case $\varepsilon \searrow 0$, the operator D goes over to the projection operator to all negative-frequency solutions (5.4). The corresponding quantum state ω is the vacuum state in the corresponding spacetime.

Remark 2.1.2. [13, Remark 2.1] (with slight modifications)

We point out that our definition of entanglement entropy differs from the conventions in [24, 30] in that we do not add the corresponding term for the complement of Λ in (1.2). This is justified as follows. On the technical level, our procedure is easier, because it suffices to consider compact spatial regions in the cases of Schwarzschild and Minkowski spacetimes (indeed, we for example expect that $\eta_{\kappa}(\chi_{\tilde{\mathcal{K}}^c} \Pi_{\text{BH}}^{(\varepsilon)} \chi_{\tilde{\mathcal{K}}^c}) - \chi_{\tilde{\mathcal{K}}^c} \eta_{\kappa}(\Pi_{\text{BH}}^{(\varepsilon)}) \chi_{\tilde{\mathcal{K}}^c}$ is not trace class). Conceptually, restricting attention to $S_{\kappa}(\Pi^{(\varepsilon)}, \Lambda)$ can be understood from the fact that occupied states which are supported either inside or outside Λ do not contribute to the entanglement entropy. Thus it suffices to consider the states which are non-zero both inside and outside. These “boundary states” are taken into account already in (1.2).

This qualitative argument can be made more precise with the following formal computation, which shows that at least for the unregularized fermionic projector (denoted by Π_-) the value of $S_{\kappa}(\Pi_-, \Lambda)$ is the same as $S_{\kappa}(\Pi_-, \Lambda^c)$: First of all note that $\eta_{\kappa}(t)$ vanishes at $t = 0$ and $t = 1$. Since Π_- is a projection this means that

$$\eta_{\kappa}(\Pi_-) = 0 \quad \text{and therefore} \quad \text{tr}(\chi_{\Lambda} \eta_{\kappa}(\Pi_-) \chi_{\Lambda}) = 0 = \text{tr}(\chi_{\Lambda^c} \eta_{\kappa}(\Pi_-) \chi_{\Lambda^c}).$$

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Moreover, if we assume that both $\chi_\Lambda \Pi_- \chi_\Lambda$ and $\Pi_- \chi_\Lambda \Pi_-$ are compact operators, we can find a one-to-one correspondence between their non-zero eigenvalues: Take any eigenvector ψ of $\chi_\Lambda \Pi_- \chi_\Lambda$ with eigenvalue $\lambda \neq 0$, then we must have

$$\chi_\Lambda \psi = \frac{1}{\lambda} \chi_\Lambda^2 \Pi_- \chi_\Lambda \psi = \psi \quad \text{and} \quad \Pi_- \psi \neq 0,$$

which yields

$$\lambda \psi = (\chi_\Lambda \Pi_- \chi_\Lambda) \psi = (\chi_\Lambda \Pi_-) \psi.$$

Then $\Pi_- \psi$ is an eigenvector of $\Pi_- \chi_\Lambda \Pi_-$ with eigenvalue λ because

$$(\Pi_- \chi_\Lambda \Pi_-)(\Pi_- \psi) = \Pi_- (\chi_\Lambda \Pi_-) \psi = \lambda \Pi_- \psi.$$

Since the same argument also works with the roles of $\Pi_- \chi_\Lambda \Pi_-$ and $\chi_\Lambda \Pi_- \chi_\Lambda$ interchanged, this shows, that the nonzero eigenvalues of both operators (counted with multiplicities) coincide. Then the same holds true for $\eta_\varkappa(\Pi_- \chi_\Lambda \Pi_-)$ and $\eta_\varkappa(\chi_\Lambda \Pi_- \chi_\Lambda)$, proving that

$$\text{tr} \eta_\varkappa(\chi_\Lambda \Pi_- \chi_\Lambda) = \text{tr} \eta_\varkappa(\Pi_- \chi_\Lambda \Pi_-).$$

Due to the symmetry of η_\varkappa , namely

$$\eta_\varkappa(t) = \eta_\varkappa(1 - t) \quad \text{for any } t \in \mathbb{R},$$

this then leads to

$$\text{tr} \eta_\varkappa(\chi_\Lambda \Pi_- \chi_\Lambda) = \text{tr} \eta_\varkappa(\Pi_- \chi_\Lambda \Pi_-) = \text{tr} \eta_\varkappa(\Pi_- - \Pi_- \chi_\Lambda \Pi_-) = \text{tr} \eta_\varkappa(\Pi_- \chi_{\Lambda^c} \Pi_-).$$

Repeating the same argument as before with $\chi_{\Lambda^c} \Pi_- \chi_{\Lambda^c}$ finally gives

$$\text{tr} \eta_\varkappa(\chi_\Lambda \Pi_- \chi_\Lambda) = \text{tr} \eta_\varkappa(\Pi_- \chi_{\Lambda^c} \Pi_-) = \text{tr} \eta_\varkappa(\chi_{\Lambda^c} \Pi_- \chi_{\Lambda^c}).$$

Regularizing this expression suggests that the entanglement entropies of the inside and outside as defined in (1.2) coincide. Then, our definition of entanglement entropy would agree (up to a numerical factor) with the one in [24, 30].

Note that the above formal computation corresponds to the fact, that for a pure bipartite state, the von Neumann entropy of both parts coincide. \diamond

2.2. Technical Preliminaries

2.2.1. Definitions

Singular Values and Schatten-von Neumann Classes

This section is based on [15, Section 4.1], [14, Section 2.3.2] and [13, Sections 2.4 and 7.1] (with similar phrasing).

Given a separable Hilbert space \mathcal{H} we denote the space of compact operators on it by \mathbf{S}_∞ . For any $A \in \mathbf{S}_\infty$ we denote by $s_k(A)$, $k = 1, 2, \dots$, its singular values i.e. eigenvalues of the self-adjoint compact operator $\sqrt{A^* A}$ labeled in non-increasing

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order counting multiplicities. For the sum $A + B$ the following inequality holds (see [7, Sec. 11.1 Eq. (14)]):

$$s_{2k}(A + B) \leq s_{2k-1}(A + B) \leq s_k(A) + s_k(B).$$

We say that A belongs to the Schatten-von Neumann class \mathbf{S}_p , $p > 0$, if

$$\|A\|_p := (\operatorname{tr} |A|^p)^{1/p} = \left(\sum_{k=1}^{\infty} s_k(A)^p \right)^{1/p} < \infty .$$

The functional $\|A\|_p$ defines a norm if $p \geq 1$ and a quasi-norm if $0 < p < 1$. With this (quasi-)norm, the class \mathbf{S}_p is a complete space (see also [7, Sections 11.4.2 and 11.5.4]). Note that for $p = 1$ this coincides with the trace norm. For $0 < p < 1$ the quasi-norm is actually a p -norm, that is, it satisfies the following ‘‘triangle inequality’’ for all $A, B \in \mathbf{S}_p$ (see [7, Section 11.5.4]):

$$\|A + B\|_p^p \leq \|A\|_p^p + \|B\|_p^p. \quad (2.4)$$

This inequality is used systematically in what follows. We point out a useful estimate for individual eigenvalues for operators in \mathbf{S}_p :¹

$$s_k(A) \leq k^{-\frac{1}{p}} \|A\|_p, \quad k = 1, 2, \dots .$$

Moreover, as explained in [7, Section 11.4.1]², for any two bounded operators B_1, B_2 on \mathcal{H} , $p > 0$ and $A \in \mathbf{S}_p$ it holds that $B_1 A B_2 \in \mathbf{S}_p$ with

$$\|B_1 A B_2\|_p \leq \|A\|_p \|B_1\|_{\infty} \|B_2\|_{\infty}, \quad (2.5)$$

and for any two $0 < p_1 < p_2 \leq \infty$, we have $\mathbf{S}_{p_1} \subset \mathbf{S}_{p_2}$ and for any $A \in \mathbf{S}_{p_1}$

$$\|A\|_{p_2} \leq \|A\|_{p_1}. \quad (2.6)$$

Finally (also according to [7, Section 11.4.1]), for any $p > 0$ and $A \in \mathbf{S}_p$, the adjoint $A^* \in \mathbf{S}_p$ with

$$\|A^*\|_p = \|A\|_p. \quad (2.7)$$

Remark 2.2.1.

- (i) Note that for any $p > 0$, the norm $\|\cdot\|_p$ is invariant under unitary transformations: Let \mathcal{H} and \mathcal{G} be separable Hilbert spaces, $U : \mathcal{G} \rightarrow \mathcal{H}$ unitary and $A \in \mathbf{S}_p \subseteq \mathbf{L}(\mathcal{H})$, then

$$(U^{-1} A U)^* U^{-1} A U = (U^* A U)^* U^{-1} A U = U^* A^* U U^{-1} A U = U^{-1} A^* A U ,$$

which is unitarily equivalent to $A^* A$ and thus has the same eigenvalues showing that

$$\|A\|_p = \|U^{-1} A U\|_p .$$

¹This follows by definition since $k s_k^p(A) \leq \sum_{l=1}^k s_l(A)^p \leq \|A\|_p^p$ (see also [7, Section 11.6.1]).

²There is a typing error in the source for (2.6), but the similarity to the l^p -spaces makes it clear.

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(ii) Let $k \in \mathbb{N}$ be a number and \mathcal{H} a separable Hilbert space. Denote \mathbf{S}_p as the p -Schatten-von Neumann class in $L(\mathcal{H}, \mathcal{H})$ and let $\mathbf{S}_p^{(k)}$ be the p -Schatten-von-Neumann class in $L(\mathcal{H}^k, \mathcal{H}^k)$. Moreover, let $A = (a_{ij})_{1 \leq i, j \leq n}$ be a formal block operator such that each block $a_{ij} \in \mathbf{S}_p$. Denote by $\tilde{a}_{i,j}$ is the block operator with zeros everywhere except for position (i, j) , where it coincides with $a_{i,j}$. Since for any $i, j \in \{1, \dots, n\}$, the operator $\tilde{a}_{i,j}^* \tilde{a}_{i,j}$ is also a formal block operator with the only non-zero entry $a_{i,j}^* a_{i,j}$ we conclude that $\tilde{a}_{i,j} \in \mathbf{S}_p^{(k)}$ and

$$\|\tilde{a}_{i,j}\|_p = \|a_{i,j}\|_p, \quad \text{for any } i, j \in \{1, \dots, n\},$$

where the norms on the left hand side are with respect to $\mathbf{S}_p^{(k)}$ and the ones on the right hand side with respect to \mathbf{S}_p . Then, applying the triangle inequality (2.4) we see that $A \in \mathbf{S}_p^{(k)}$ as well and its p -norm can be estimated by

$$\|A\|_p^p \leq \sum_{i=1}^n \sum_{j=1}^n \|\tilde{a}_{i,j}\|_p^p = \sum_{i=1}^n \sum_{j=1}^n \|a_{i,j}\|_p^p,$$

where the norms on the very left hand side are with respect to $\mathbf{S}_p^{(k)}$ and on the very right hand side with respect to \mathbf{S}_p .

◇

We refer to [7, Chapter 11] for more details on singular values.

Pseudo-differential Operators

This section is based on [13, Sections 3.3 and 6.2], [14, Section 2.3.1] and [15, Section 1] (with similar phrasing).

Let $n, d \in \mathbb{N}$ be two parameters. We will often rewrite operators on $L^2(\mathbb{R}^d, \mathbb{C}^n)$ as Pseudo-differential operators of the form

$$\left(\text{Op}_\alpha(\mathcal{A})\psi\right)(\mathbf{x}) := \left(\frac{\alpha}{2\pi}\right)^d \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} e^{-i\alpha\xi \cdot (\mathbf{x}-\mathbf{y})} \mathcal{A}(\mathbf{x}, \mathbf{y}, \xi) \psi(\mathbf{y}) d\mathbf{y} d\xi \quad (2.8)$$

for any $\psi \in C_0^\infty(\mathbb{R}^d, \mathbb{C}^n)$.

The so called *symbol* \mathcal{A} is a suitable measurable matrix-valued map $\mathcal{A} : (\mathbb{R}^d)^3 \rightarrow \mathbb{C}^{n \times n}$ such that the operator on $C_0^\infty(\mathbb{R}^d, \mathbb{C}^n)$ defined by (2.8) can be extended continuously to all of $L^2(\mathbb{R}^d, \mathbb{C}^n)$. The parameter $d \in \mathbb{N}$ can be thought of as the spatial dimension and the parameter $n \in \mathbb{N}$ as the number of components of the wave function ψ .

Note that symbols denoted with lowercase letters in this thesis usually indicate that the symbol is scalar-valued.

Moreover, the symbols sometimes additionally depend on ε or other parameters. We usually denote this by corresponding super- or subscripts.

For some symbols \mathcal{A} the integral representation (2.8) extends to all Schwartz- or even all L^2 -functions. If this condition is assumed for specific results, we will mention it explicitly. We will also establish some conditions on \mathcal{A} that guarantee such extensions.

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The notation of the arguments of the symbol \mathcal{A} is often adapted to the application in mind. In particular, if the arguments are *not* boldface this usually implies that they are scalar-valued, i.e. $d = 1$.

Furthermore, note that for any measurable set $U \subset \mathbb{R}^d$ we can identify $\text{Op}_\alpha(\mathcal{A})$ as an operator on $L^2(U, \mathbb{C}^n)$ by restricting the \mathbf{y} -integral in (2.8) to U and only evaluating for $\mathbf{x} \in U$. Moreover, given an operator on $L^2(U, \mathbb{C}^n)$ with integral representation (2.8) but with the \mathbf{y} -integral restricted to U , we can identify it with a pseudo-differential operator on $L^2(\mathbb{R}^d, \mathbb{C}^n)$ by integrating in \mathbf{y} over all of \mathbb{R}^d and replacing $\mathcal{A}(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi})$ with $\chi_U(\mathbf{x})\mathcal{A}(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi})\chi_U(\mathbf{y})$. We will sometimes make use of this identification later on without specifically mentioning it.

For self-adjoint operators $\text{Op}_\alpha(\mathcal{A})$ we recall the definition of $D_\alpha(\eta, \Lambda, \mathcal{A})$ from (1.9):

$$D_\alpha(f, \Lambda, \mathcal{A}) = f(\chi_\Lambda \text{Op}_\alpha(\mathcal{A})\chi_\Lambda) - \chi_\Lambda f(\text{Op}_\alpha(\mathcal{A}))\chi_\Lambda,$$

where $\Lambda \subseteq \mathbb{R}^d$ is some measurable set which will be specified later and f is a measurable function on the spectrum of $\text{Op}_\alpha(\mathcal{A})$. For technical purposes it is also useful to introduce the truncated operator:

$$W_\alpha(\mathcal{A}, \Lambda) := \chi_\Lambda \text{Op}_\alpha(\mathcal{A})\chi_\Lambda.$$

Moreover, in what follows we will often use the notation

$$P_{\Omega, \alpha} := \text{Op}_\alpha(\chi_\Omega)$$

for some measurable set $\Omega \subseteq \mathbb{R}^d$, which emphasizes that this is a projection operator (this and its well-definedness will follow from Lemma 3.0.1). In Lemma 3.0.2 we will see that the integral representation of such operators always extends to all Schwartz functions.

Norms on Symbols and Functions

This section is based on [13, Definition 2.7] and [15, Section 4.2] (with similar phrasing).

We will frequently use the following function norms.

Definition 2.2.2. (see for example [39, Section 2.1] with slight modifications)

Let $\mathbf{S}^{(j,k,l)}(\mathbb{R}^d)$ with $j, k, l \in \mathbb{N}_0$ be the space of all complex-valued functions on $(\mathbb{R}^d)^3$, which are continuous, bounded and continuously partially differentiable in the first variable up to order j , in the second to k and in the third to l and whose partial derivatives up to these orders are bounded as well. For $a \in \mathbf{S}^{(j,k,l)}(\mathbb{R}^d)$ and $s, \delta > 0$ we introduce the norm

$$\mathbf{N}^{(j,k,l)}(a; s, \delta) := \max_{\substack{0 \leq \tilde{j} \leq j \\ 0 \leq \tilde{k} \leq k \\ 0 \leq \tilde{l} \leq l}} \sup_{\mathbf{x}, \mathbf{y}, \boldsymbol{\xi}} s^{\tilde{j} + \tilde{k}} \delta^{\tilde{l}} |\nabla_{\mathbf{x}}^{\tilde{j}} \nabla_{\mathbf{y}}^{\tilde{k}} \nabla_{\boldsymbol{\xi}}^{\tilde{l}} a(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi})|.$$

Similarly, $\mathbf{S}^{(j,l)}(\mathbb{R}^d)$ with $j, l \in \mathbb{N}_0$ denotes the space of all complex-valued functions on $(\mathbb{R}^d)^2$, which are continuous and bounded and continuously partially differentiable in

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the first variable up to order j and in the second to l and whose partial derivatives up to these orders are bounded. For $a \in \mathbf{S}^{(j,l)}(\mathbb{R}^d)$ and $s, \delta > 0$ we introduce the norm

$$\mathbf{N}^{(j,l)}(a; s, \delta) := \max_{\substack{0 \leq \bar{j} \leq j \\ 0 \leq \bar{l} \leq l}} \sup_{\mathbf{x}, \boldsymbol{\xi}} s^{\bar{j}} \delta^{\bar{l}} |\nabla_{\mathbf{x}}^{\bar{j}} \nabla_{\boldsymbol{\xi}}^{\bar{l}} a(\mathbf{x}, \boldsymbol{\xi})|.$$

Finally, by $\mathbf{S}^{(l)}(\mathbb{R}^d)$ with $l \in \mathbb{N}_0$ we denote the space of all complex-valued functions on \mathbb{R}^d , which are continuous and bounded and continuously partially differentiable up to order l and whose partial derivatives up to this order are bounded. For $a \in \mathbf{S}^{(l)}(\mathbb{R}^d)$ and $\delta > 0$ we introduce the norm

$$\mathbf{N}^{(l)}(a; \delta) := \max_{0 \leq \bar{l} \leq l} \sup_{\boldsymbol{\xi}} \delta^{\bar{l}} |\nabla_{\boldsymbol{\xi}}^{\bar{l}} a(\boldsymbol{\xi})|.$$

Note that any function $a \in \mathbf{S}^{(j,l)}(\mathbb{R}^d)$ may be interpreted as element of in $\mathbf{S}^{(j,k,l)}(\mathbb{R}^d)$ for any $k \in \mathbb{N}_0$ by the identification

$$a(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi}) \equiv a(\mathbf{x}, \boldsymbol{\xi}) \quad \text{for any } \mathbf{y} \in \mathbb{R}^d.$$

Then, for any $s, \delta > 0$ one has

$$\mathbf{N}^{(j,k,l)}(a; s, \delta) = \mathbf{N}^{(j,l)}(a; s, \delta).$$

And similarly for $a \in \mathbf{S}^{(l)}(\mathbb{R}^d)$.

Another useful functional is given as follows.

Definition 2.2.3. (see [40, Section 2.1] with similar phrasing)

Let $\mathcal{C} = [0, 1]^d$ and for any $\mathbf{u} \in \mathbb{R}^d$ set $\mathcal{C}_{\mathbf{u}} := \mathcal{C} + \mathbf{u}$. Let $h \in \mathbf{L}_{\text{loc}}^r(\mathbb{R}^d)$ and $p \in (0, \infty)$, then we denote

$$\begin{cases} |h|_{p,\delta} = \left[\sum_{\mathbf{n} \in \mathbb{Z}^d} \left(\int_{\mathcal{C}_{\mathbf{n}}} |h(\mathbf{x})|^p d\mathbf{x} \right)^{\frac{\delta}{p}} \right]^{\frac{1}{\delta}}, & 0 < \delta < \infty, \\ |h|_{p,\infty} = \sup_{\mathbf{u} \in \mathbb{R}^d} \left(\int_{\mathcal{C}_{\mathbf{u}}} |h(\mathbf{x})|^p d\mathbf{x} \right)^{\frac{1}{p}}, & \delta = \infty. \end{cases}$$

Sometimes these functionals are called **lattice quasi-norms** (norms for $p, \delta \geq 1$). We say $h \in \mathbf{l}^{\delta}(\mathbf{L}^p)(\mathbb{R}^d)$ if $|h|_{p,\delta} < \infty$.

2.2.2. Abstract Estimates

In this section we list a few (mostly) previously established results, which can mostly also be found in a similar (or sometimes same) form and phrasing in several chapters of the works [13], [14] and [15].

Consider an arbitrary separable Hilbert space \mathcal{H} . Let A be a bounded self-adjoint operator and let P be an orthogonal projection on \mathcal{H} . Given a measurable function³ f we define the operator

$$D(A, P; f) := Pf(PAP)P - Pf(A)P. \tag{2.9}$$

³We use the convention that if the function is initially not defined on the entire spectrum of A , we simply extend it by 0.

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Sometimes for ease of notation we leave out some of the arguments of D , i.e. we sometimes write $D(A; f) \equiv D(A, P; f)$ or $D(A) \equiv D(A, P; f)$.

In the following we establish a few estimates for this operator.

Theorem 2.2.4. [41, Corollary 2.11] (Simplified and adapted to our notation)
 Let \mathcal{H} be a separable Hilbert space, $q, R > 0$ parameters, $k \geq 2$ a natural number and $f \in C_0^k(-R, R)$. Let $\sigma \in (0, 1]$ such that

$$(k - \sigma)^{-1} < q \leq 1.$$

Given a bounded self-adjoint operator A on \mathcal{H} and an orthogonal projection P on \mathcal{H} such that $PA(I - P) \in \mathbf{S}_{\sigma q}$, the following estimate holds

$$\|f(PAP)P - Pf(A)\|_q \lesssim \max_{0 \leq j \leq k} \left(R^j \|f^{(j)}\|_{L^\infty} \right) R^{-\sigma} \|PA(\mathbf{1} - P)\|_{\sigma q}^\sigma$$

with an implicit constant independent of A, P, f and R .⁴

In what follows it is convenient to require that the function f satisfies the following condition, which can for example be found in [41, Theorem 4.4] (with similar phrasing).

Condition 2.2.5. Let $\mathbb{T} := \{t_0, \dots, t_K\}$ be a finite set and $g \in C^2(\mathbb{R} \setminus \mathbb{T}) \cap C^0(\mathbb{R})$ be a function such that there exists a constant $\gamma > 0$ and in the neighborhood of every t_i there are constants $c_k > 0$, $k = 0, 1, 2$ satisfying the conditions

$$|g^{(k)}(x)| \leq c_k |t - t_i|^{\gamma - k}.$$

For technical purposes we will also make use of the following related condition.

Condition 2.2.6. [15, Condition 5.1] The function $f \in C^2(\mathbb{R} \setminus \{t_0\}) \cap C(\mathbb{R})$ satisfies the bound

$$\|f\|_2 := \max_{0 \leq k \leq 2} \sup_{t \neq t_0} |f^{(k)}(t)| |t - t_0|^{-\gamma + k} < \infty$$

for some $\gamma \in (0, 1]$, and it is supported on the interval $(t_0 - R, t_0 + R)$ with some finite $R > 0$.

Remark 2.2.7. Note that if \mathbb{T} contains only one element, the two conditions coincide. Moreover, if f satisfies Condition 2.2.5 and $(\psi_k)_{0 \leq k \leq l}$ is suitable partition of unity such that the support of each ψ_k only contains exactly one of the elements in \mathbb{T} , then each $f\psi_k$ satisfies Condition 2.2.6. \diamond

Example 2.2.8. As shown in detail in Lemma C.0.1, for any $\varkappa \neq 1$, the Rényi entropy function η_\varkappa satisfies Condition 2.2.5 with $\mathbb{T} = \{0, 1\}$ for any $\gamma \leq \min\{\varkappa, 1\}$. Moreover, $\eta = \eta_1$ satisfies Condition 2.2.5 with $\mathbb{T} = \{0, 1\}$ for any $\gamma < 1$. \diamond

The next proposition follows from a more general fact proven in [41, Theorem 2.4], see also [31, Proposition 2.2] (note that we used similar phrasing).

⁴The independence on f and R is not explicitly stated in [41, Corollary 2.11], but [41, Corollary 2.7] plus the proofs of both corollaries make it clear.

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Proposition 2.2.9. *Suppose that f satisfies Condition 2.2.6 with some $\gamma \in (0, 1]$ and some $t_0 \in \mathbb{R}$, $R > 0$. Let $q \in (1/2, 1]$ and assume that $\sigma < \min\{2 - q^{-1}, \gamma\}$. Let A be a bounded self-adjoint operator on a separable Hilbert space \mathcal{H} and let P be an orthogonal projection on \mathcal{H} such that $PA(\mathbb{1} - P) \in \mathbf{S}_{\sigma q}$. Then*

$$\|D(A, P; f)\|_q \lesssim \|f\|_2 R^{\gamma-\sigma} \|PA(\mathbb{1} - P)\|_{\sigma q}^\sigma,$$

with an implicit constant independent of A , P , f , R and t_0 .

Applying Proposition 2.2.9 with

$$A = \text{Op}_\alpha(\mathcal{A}), \quad P = \chi_\Lambda,$$

we obtain the following Corollary (we again use similar phrasing as in [41, Theorem 2.4] and [31, Proposition 2.2]).

Corollary 2.2.10. *Suppose that f satisfies Condition 2.2.6 with some $\gamma \in (0, 1]$ and some $t_0 \in \mathbb{R}$, $R > 0$. Let $q \in (1/2, 1]$ and assume that $\sigma < \min\{2 - q^{-1}, \gamma\}$. Let \mathcal{A} be a bounded, Hermitian matrix-valued symbol and $\Lambda \subset \mathbb{R}^d$ such that the operator $\chi_\Lambda \text{Op}_\alpha(\mathcal{A})(1 - \chi_\Lambda) \in \mathbf{S}_{\sigma q}$. Then*

$$\|D_\alpha(\mathcal{A}, \chi_\Lambda; f)\|_q \lesssim \|f\|_2 R^{\gamma-\sigma} \|\chi_\Lambda \text{Op}_\alpha(\mathcal{A})(1 - \chi_\Lambda)\|_{\sigma q}^\sigma, \quad (2.10)$$

with a positive implicit constant independent of \mathcal{A} , Λ , the function f and the parameter R .

In order to estimate the Schatten norm on the right hand side of (2.10), we will sometimes use estimates of the Schatten norm of the commutator $[\chi_\Lambda, \text{Op}_\alpha(\mathcal{A})]$. The next Lemma shows that this is indeed equivalent.

Lemma 2.2.11. *Let $0 < p < 1$ and \mathcal{H} a separable Hilbert space.*

(i) *If A, B are bounded self-adjoint operators on \mathcal{H} such that $BA(\mathbb{1} - B) \in \mathbf{S}_p$, then also $[A, B] \in \mathbf{S}_p$ and*

$$\|[A, B]\|_p \leq 2\|BA(\mathbb{1} - B)\|_p.$$

(ii) *If B is a projection on \mathcal{H} and A some operator on \mathcal{H} such that $[A, B] \in \mathbf{S}_p$, then also $BA(\mathbb{1} - B) \in \mathbf{S}_p$ and*

$$\|BA(\mathbb{1} - B)\|_p \leq \|[A, B]\|_p$$

Proof. (i): We apply the triangle inequality,

$$\begin{aligned} \|[A, B]\|_p^p &= \|AB - BAB + BAB - BA\|_p^p = \|(\mathbb{1} - B)AB - BA(\mathbb{1} - B)\|_p^p \\ &\leq \|(\mathbb{1} - B)AB\|_p^p + \|BA(\mathbb{1} - B)\|_p^p \leq 2\|BA(\mathbb{1} - B)\|_p^p \end{aligned}$$

where we also used that

$$((\mathbb{1} - B)AB)^* = BA(\mathbb{1} - B),$$

together with (2.7).

(ii): We make use of (2.5) and the fact that B is a projection,

$$\|BA - BAB\|_p = \|B(BA - AB)\|_p \leq \|B\|_\infty \|[A, B]\|_p \leq \|[A, B]\|_p.$$

□

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2.2.3. Estimates for Pseudo-Differential Operators

In this section we list a few previously established results, which can also be found in a similar (or sometimes same) form and phrasing in several chapters of the works [13], [14] and [15].

The first lemma shows that $\text{Op}_\alpha(a)$ is bounded with respect to the operator norm uniformly in α as long as the symbol a is suitably regular.

Lemma 2.2.12. [39, Lemma 3.9] (with slight modifications)

Let $k := \lfloor d/2 \rfloor + 1$ be a parameter, $\alpha_0 > 0$ a constant and $s, \delta > 0$ such that $\alpha s \delta \geq \alpha_0$. Moreover, let $a \in \mathbf{S}^{(k, k, d+1)}(\mathbb{R}^d)$ be a symbol. Assume that $\text{Op}_\alpha(a)$ is well defined, its integral representation extends to all Schwartz functions and the \mathbf{y} - and $\boldsymbol{\xi}$ -integrals in the integral representation are interchangeable for any Schwartz function. Then

$$\|\text{Op}_\alpha(a)\|_\infty \lesssim \mathbf{N}^{(k, k, d+1)}(a; s, \delta),$$

with an implicit constant only depending on d and α_0 .

Proposition 2.2.13. [39, Proposition 3.8] with reference to [6, Theorem 11.1], [5, Section 5.8] and [38, Theorem 4.5] (with slight modifications)⁵

Let $a, h \in \mathcal{L}^q(\mathbb{L}^2)(\mathbb{R}^m)$ for some $q \in (0, 2)$. Assume that the integral representation of $\text{Op}_1(a)$ extends to all Schwartz functions and that the \mathbf{y} - and $\boldsymbol{\xi}$ -integrals in the integral representation are interchangeable for any Schwartz function. Then $h \text{Op}_1(a) \in \mathbf{S}_q$ and

$$\|h \text{Op}_1(a)\|_q \lesssim \|h\|_{2, q} \|a\|_{2, q},$$

with an implicit constant independent of a and h .

The next Corollary helps us to estimate the error caused by interchanging characteristic functions in position and momentum space.

Corollary 2.2.14. [40, Corollary 4.7] (case $d = 1$, with slight modifications)

For any two open bounded intervals $K, J \subset \mathbb{R}$ as well as numbers $q \in (0, 1]$ and $\alpha \geq 2$, the following estimate holds,

$$\|\chi_K P_{J, \alpha}(1 - \chi_K)\|_q \lesssim (\ln \alpha)^{1/q},$$

with an implicit constant independent of $\alpha \geq 2$.

The next proposition gives an estimate for terms of the form $\|\chi_\Lambda \text{Op}_\alpha(a)(1 - \chi_\Lambda)\|_q$, which will come up when applying Theorem 2.2.4 or Proposition 2.2.9. It follows from the more general result [31, Proposition 3.2] (see also [40, Corollary 4.4]). We adapted it to the cases needed and to our notation, moreover the coefficient in k was corrected (in comparison to the version in [31, Proposition 3.2]), after talking it over with one of the authors (Alexander V. Sobolev).

Proposition 2.2.15. Let $d = 1$ and $K \subset \mathbb{R}$ be an open bounded interval and let $\alpha_0 > 0$ be a constant. Let $q \in (0, 1]$ and

$$k = \lfloor 2q^{-1} \rfloor + 1.$$

⁵There is a typing error in [39, Proposition 3.8], but [6, Theorem 11.1] makes it clear.

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Let a be a scalar-valued symbol independent of x and y , i.e. $a(x, y, \xi) \equiv a(\xi)$ with support contained in $B_\delta(\zeta)$ for some $\zeta \in \mathbb{R}$ and $\delta > 0$. Assume that $a \in \mathbf{S}^{(k)}(\mathbb{R})$ and $\text{Op}_\alpha(a)$ is well defined with integral representation extending to all Schwartz functions. Then for any $\alpha\delta \geq \alpha_0$,

$$\|\chi_K \text{Op}_\alpha(a)(1 - \chi_K)\|_q \lesssim \mathbf{N}^{(k)}(a; \delta),$$

with implicit constants independent of a , α , δ and ζ .

3. Further Properties of Pseudo-Differential Operators

This section is based on [13, Section 5] and [14, Section 2.3.1] (with similar phrasing). We establish a few general results for pseudo-differential operators.

Lemma 3.0.1. *Let \mathcal{A} be a Hermitian matrix-valued symbol which is measurable, independent of \mathbf{x} and \mathbf{y} , i.e. $\mathcal{A}(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi}) \equiv \mathcal{A}(\boldsymbol{\xi})$ and bounded in $\boldsymbol{\xi}$, then $\text{Op}_\alpha(\mathcal{A})$ is well-defined and self-adjoint. Moreover, for any Borel function f defined on the spectrum of $\text{Op}_\alpha(\mathcal{A})$, we have*

$$f(\text{Op}_\alpha(\mathcal{A})) = \text{Op}_\alpha(f(\mathcal{A})) .$$

Proof. Note that for a symbol \mathcal{A} as in the claim

$$\text{Op}_\alpha(\mathcal{A}) = \mathcal{F} \mathcal{A}(\cdot/\alpha) \mathcal{F}^{-1} , \tag{3.1}$$

since (3.1) holds for all $C_0^\infty(\mathbb{R}^d, \mathbb{C}^n)$ -functions and the right hand side defines a bounded operator on $L^2(\mathbb{R}^d, \mathbb{C}^n)$. This also shows, that $\text{Op}_\alpha(\mathcal{A})$ is bounded (and therefore well-defined) and self-adjoint. Since for any $\boldsymbol{\xi} \in \mathbb{R}^d$, the matrix $\mathcal{A}(\boldsymbol{\xi}/\alpha)$ is Hermitian matrix-valued the spectral theorem for matrices yields a unitary matrix $\mathcal{V}(\boldsymbol{\xi})$ such that

$$\mathcal{V}(\boldsymbol{\xi})\mathcal{A}(\boldsymbol{\xi}/\alpha)\mathcal{V}(\boldsymbol{\xi})^{-1} = \text{diag}(b_1(\boldsymbol{\xi}), \dots, b_n(\boldsymbol{\xi})) =: \mathcal{B}(\boldsymbol{\xi}) .$$

Then, using the identification $L^2(\mathbb{R}^d, \mathbb{C}^n) \cong L^2(\{1, \dots, n\} \times \mathbb{R}^d, \mathbb{C})$, the operator $\mathcal{V}(\cdot)^{-1}\mathcal{F}^{-1}$ can be interpreted as the unitary transformation from the multiplicative version of the spectral theorem for the operator $\text{Op}_\alpha(\mathcal{A})$ and \mathcal{B} as the corresponding function. Thus we have

$$f(\text{Op}_\alpha(\mathcal{A})) = \mathcal{F} \mathcal{V}(\cdot) f(\mathcal{B}(\cdot/\alpha)) \mathcal{V}(\cdot)^{-1} \mathcal{F}^{-1} = \mathcal{F} f(\mathcal{A}(\cdot/\alpha)) \mathcal{F}^{-1} = \text{Op}_\alpha(f(\mathcal{A})) .$$

□

A similar argument as in the above proof can be used to prove a criterion on when the integral representation of $\text{Op}_\alpha(\mathcal{A})$ extends to all Schwartz functions.

Lemma 3.0.2. *Let \mathcal{A} be a symbol which is independent of \mathbf{x} and \mathbf{y} such that for any Schwartz function $\psi \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^n)$, the vector-valued function $\mathcal{A}(\cdot/\alpha)\psi(\cdot) \in L^1(\mathbb{R}^d, \mathbb{C}^n)$, then the integral representation of $\text{Op}_\alpha(\mathcal{A})$ extends to all Schwartz functions. In particular this holds for any measurable symbol \mathcal{A} which is independent of \mathbf{x} and \mathbf{y} and bounded in $\boldsymbol{\xi}$.*

Proof. Just as in the proof of Lemma 3.0.1 we conclude that

$$\text{Op}_\alpha(\mathcal{A}) = \mathcal{F}^{-1} \mathcal{A}(\cdot/\alpha) \mathcal{F} .$$

3. Further Properties of Pseudo-Differential Operators

Now take an arbitrary Schwartz function $\psi \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^n)$, then $\mathcal{F}\psi$ is defined by the usual integral representation. Moreover we have $\mathcal{F}\psi \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^n)$, since \mathcal{F} is an automorphism on the Schwartz space. Furthermore, since the map $\boldsymbol{\xi} \mapsto \mathcal{A}(\boldsymbol{\xi}/\alpha)(\mathcal{F}\psi)(\boldsymbol{\xi})$ is in $L^1(\mathbb{R}^d, \mathbb{C}^n)$, the inverse Fourier transform is again given by the usual integral representation meaning that the integral representation of $\text{Op}_\alpha(\mathcal{A})$ extends to ψ . Since $\psi \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^n)$ was chosen arbitrarily, the claim follows. \square

The next lemma will be needed for consistency reasons when considering the limit $u_0 \rightarrow -\infty$:

Lemma 3.0.3. *Let $\text{Op}_\alpha(\mathcal{A})$ as in Section 2.2.1, let $U, V \subset \mathbb{R}^d$ be arbitrary Borel sets and $\mathbf{c} \in \mathbb{R}^d$ an arbitrary vector. For any $\mathbf{x}, \mathbf{y}, \boldsymbol{\xi} \in \mathbb{R}^d$ we transform a given symbol \mathcal{A} by*

$$T_{\mathbf{c}}(\mathcal{A})(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi}) := \mathcal{A}(\mathbf{x} + \mathbf{c}, \mathbf{y} + \mathbf{c}, \boldsymbol{\xi}).$$

Then there is a unitary transformation $t_{\mathbf{c}}$ on $L^2(\mathbb{R}^d, \mathbb{C}^n)$ such that

$$t_{\mathbf{c}} \chi_{U+\mathbf{c}} \text{Op}_\alpha(T_{-\mathbf{c}}(\mathcal{A})) \chi_{V+\mathbf{c}} t_{\mathbf{c}}^{-1} = \chi_U \text{Op}_\alpha(\mathcal{A}) \chi_V. \quad (3.2)$$

Moreover, assuming in addition that $\text{Op}_\alpha(\mathcal{A})$ is self-adjoint, we conclude that for any Borel function f on the spectrum of \mathcal{A} ,

$$f(\chi_U \text{Op}_\alpha(\mathcal{A}) \chi_U) = t_{\mathbf{c}} f(\chi_{U+\mathbf{c}} \text{Op}_\alpha(T_{-\mathbf{c}}(\mathcal{A})) \chi_{U+\mathbf{c}}) t_{\mathbf{c}}^{-1}. \quad (3.3)$$

Proof. We will show that the desired unitary operator is given by the translation operator

$$t_{\mathbf{c}} : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d), \quad f \mapsto f(\cdot + \mathbf{c}),$$

(which is obviously unitary). Note that for any Borel set $W \subseteq \mathbb{R}^d$

$$\chi_{W+\mathbf{c}} = t_{-\mathbf{c}} \chi_W t_{\mathbf{c}}, \quad (3.4)$$

and therefore

$$\chi_U \text{Op}_\alpha(\mathcal{A}) \chi_V = t_{\mathbf{c}} \chi_{U+\mathbf{c}} t_{-\mathbf{c}} \text{Op}_\alpha(\mathcal{A}) t_{\mathbf{c}} \chi_{V+\mathbf{c}} t_{-\mathbf{c}}.$$

By a change of variables we obtain for arbitrary $\psi \in C_0^\infty(\mathbb{R}^d, \mathbb{C}^n)$

$$\begin{aligned} & (t_{-\mathbf{c}} \text{Op}_\alpha(\mathcal{A}) t_{\mathbf{c}}\psi)(\mathbf{x}) \\ &= (\text{Op}_\alpha(\mathcal{A}) t_{\mathbf{c}}\psi)(\mathbf{x} - \mathbf{c}) = \frac{\alpha^d}{(2\pi)^d} \int d\boldsymbol{\xi} \int d\mathbf{y} e^{-i\alpha\boldsymbol{\xi}(\mathbf{x}-\mathbf{c}-\mathbf{y})} \mathcal{A}(\mathbf{x} - \mathbf{c}, \mathbf{y}, \boldsymbol{\xi}) \psi(\mathbf{y} + \mathbf{c}) \\ &= \frac{\alpha^d}{(2\pi)^d} \int d\boldsymbol{\xi} \int d\mathbf{y} e^{-i\alpha\boldsymbol{\xi}(\mathbf{x}-\mathbf{y})} \mathcal{A}(\mathbf{x} - \mathbf{c}, \mathbf{y} - \mathbf{c}, \boldsymbol{\xi},) \psi(\mathbf{y}) = (\text{Op}_\alpha(T_{-\mathbf{c}}(\mathcal{A}))\psi)(\mathbf{x}). \end{aligned}$$

This shows (3.2).

For (3.3) we make use the multiplication operator version of the spectral theorem. This provides a unitary transformation \mathcal{V} and a suitable function g such that

$$\chi_U \text{Op}_\alpha(\mathcal{A}) \chi_U = \mathcal{V}^{-1} g \mathcal{V}.$$

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Combined with the previous discussion this implies

$$\chi_{U+c} \text{Op}_\alpha(T_{-c}(\mathcal{A})) \chi_{U+c} = (\mathcal{V} t_c)^{-1} g (\mathcal{V} t_c),$$

which is the multiplication operator representation of $\chi_{U+c} \text{Op}_\alpha(T_{-c}(\mathcal{A})) \chi_{U+c}$, because $\mathcal{V} t_c$ is also a unitary operator. Therefore

$$f(\chi_{U+c} \text{Op}_\alpha(T_{-c}(\mathcal{A})) \chi_{U+c}) = (\mathcal{V} t_c)^{-1} (f \circ g) (\mathcal{V} t_c) = t_c^{-1} f(\chi_U \text{Op}_\alpha(\mathcal{A}) \chi_U) t_c,$$

concluding the proof. \square

Remark 3.0.4. A similar result as Lemma 3.0.3 holds for translations in the ξ -variable: Let $\mathbf{c} \in \mathbb{R}^d$ be an arbitrary vector. For any $\mathbf{x}, \mathbf{y}, \boldsymbol{\xi} \in \mathbb{R}^d$ we transform a given symbol \mathcal{A} by

$$R_{\mathbf{c}}(\mathcal{A})(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi}) := \mathcal{A}(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi} + \mathbf{c}).$$

Then, for any $\psi \in C_0^\infty(\mathbb{R}^d, \mathbb{C}^n)$ and $\mathbf{x} \in \mathbb{R}^d$ we have

$$\begin{aligned} (\text{Op}_\alpha(R_{\mathbf{c}}(\mathcal{A}))\psi)(\mathbf{x}) &= \frac{\alpha^d}{(2\pi)^d} \int_{\mathbb{R}^d} d\boldsymbol{\xi} \int_{\mathbb{R}^d} d\mathbf{y} e^{-i\alpha\boldsymbol{\xi}(\mathbf{x}-\mathbf{y})} \mathcal{A}(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi} + \mathbf{c}) \psi(\mathbf{y}) \\ &= \frac{\alpha^d}{(2\pi)^d} \int_{\mathbb{R}^d} d\boldsymbol{\xi} \int_{\mathbb{R}^d} d\mathbf{y} e^{-i\alpha(\boldsymbol{\xi}-\mathbf{c})(\mathbf{x}-\mathbf{y})} \mathcal{A}(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi}) \psi(\mathbf{y}) \\ &= \frac{\alpha^d}{(2\pi)^d} e^{-i\alpha\mathbf{c}\mathbf{x}} \int_{\mathbb{R}^d} d\boldsymbol{\xi} \int_{\mathbb{R}^d} d\mathbf{y} e^{-i\alpha\boldsymbol{\xi}(\mathbf{x}-\mathbf{y})} \mathcal{A}(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi}) e^{i\alpha\mathbf{c}\mathbf{y}} \psi(\mathbf{y}). \end{aligned}$$

Denoting the function $f(\mathbf{x}) := e^{i\alpha\mathbf{c}\mathbf{x}}$, this shows that

$$\text{Op}_\alpha(R_{\mathbf{c}}(\mathcal{A})) = f \text{Op}_\alpha(\mathcal{A}) f^{-1},$$

which implies similar consequences for trace and Schatten-norms since the multiplication by f is a unitary operator. \diamond

The following result can (at least for scalar-valued symbols) also be found in [39, Eq. (2.10)] using a slightly different notation and a slightly different definition of $\text{Op}_\alpha(\cdot)$. Nevertheless we decided it would be helpful to give a proof and reformulate it here.

Lemma 3.0.5. *Let \mathcal{A} be a symbol such that $\text{Op}_\alpha(\mathcal{A})$ is well defined on $L^2(\mathbb{R}^d, \mathbb{C}^n)$, let $\Lambda \subset \mathbb{R}$ be some measurable set and $\alpha, \delta > 0$ some arbitrary constants. Then,*

(i) *There is a unitary operator V_δ on $L^2(\mathbb{R}^d, \mathbb{C}^n)$ such that*

$$V_\delta^{-1} \chi_\Lambda \text{Op}_\alpha(\mathcal{A}) \chi_\Lambda V_\delta = \chi_{\delta\Lambda} \text{Op}_{\alpha/\delta}(\mathcal{A}) \chi_{\delta\Lambda}.$$

*We refer to this as **rescaling in position space**.*

(ii) *By **rescaling in momentum space** we mean the equality*

$$\text{Op}_\alpha(\mathcal{A}) = \text{Op}_{\delta\alpha}(\mathcal{A}(\delta \cdot)).$$

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Proof. First, (ii) simply follows by changing coordinates in the $\boldsymbol{\xi}$ -integral.

For (i) consider the unitary operator V_δ , which is for any $\psi \in L^2(\mathbb{R}^d, \mathbb{C}^n)$ defined by

$$(V_\delta \varphi)(\mathbf{x}) := \delta^{d/2} \psi(\delta \mathbf{x}), \quad \text{for any } \mathbf{x} \in \mathbb{R}^d.$$

Then, for any $\psi \in L^2(\mathbb{R}^d, \mathbb{C}^n)$ and $\mathbf{x} \in \mathbb{R}^d$,

$$(V_\delta^{-1} \chi_\Lambda V_\delta \psi)(\mathbf{x}) = \delta^{d/2} (V_\delta^{-1} \chi_\Lambda \psi(\delta \cdot))(\mathbf{x}) = \chi_\Lambda(\mathbf{x}/\delta) \psi(\mathbf{x}) = (\chi_{\delta\Lambda} \psi)(\mathbf{x})$$

and for any $\psi \in S(\mathbb{R}^d, \mathbb{C}^n)$

$$\begin{aligned} (V_\delta^{-1} \text{Op}_\alpha(\mathcal{A}) V_\delta \psi)(\mathbf{x}) &= \frac{\alpha^d}{2\pi} \int_{-\infty}^{\infty} d\boldsymbol{\xi} \int_{-\infty}^{\infty} d\mathbf{y} e^{i\alpha \boldsymbol{\xi} \cdot (\mathbf{x}/\delta - \mathbf{y})} \mathcal{A}(\boldsymbol{\xi}) \psi(\delta \mathbf{y}) \\ &= \frac{(\alpha/\delta)^d}{2\pi} \int_{-\infty}^{\infty} d\boldsymbol{\xi} \int_{-\infty}^{\infty} d\mathbf{y} e^{i\alpha/\delta \boldsymbol{\xi} \cdot (\mathbf{x} - \mathbf{y})} \mathcal{A}(\boldsymbol{\xi}) \psi(\mathbf{y}) = (\text{Op}_{\alpha/\delta}(\mathcal{A}) \psi)(\mathbf{x}), \end{aligned}$$

where in the second step we applied a change of variables in the \mathbf{y} -integral. \square

Lemma 3.0.6. *Let $\text{Op}_\alpha(\mathcal{A})$ as in Section 2.2.1, such that \mathcal{A} satisfies*

$$\int_{\mathbb{R}^d} d\boldsymbol{\xi} \sqrt{\int_{\mathbb{R}^d} d\mathbf{y} \|\mathcal{A}(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi})\|_{n \times n}^2} < \infty, \quad \text{for any } \mathbf{x} \in \mathbb{R}^d$$

(where $\|\cdot\|_{n \times n}$ is the ordinary sup-norm on the $n \times n$ -matrices). Then the integral-representation of $\text{Op}_\alpha(\mathcal{A})$ may be extended to all $L^2(\mathbb{R}^d, \mathbb{C}^n)$ -functions and the \mathbf{y} and the $\boldsymbol{\xi}$ integrations may be interchanged. Thus for any $\psi \in L^2(\mathbb{R}^d, \mathbb{C}^n)$ and almost any $\mathbf{x} \in \mathbb{R}^d$, the following equations hold,

$$\begin{aligned} (\text{Op}_\alpha(\mathcal{A}) \psi)(\mathbf{x}) &= \left(\frac{\alpha}{2\pi}\right)^d \int_{\mathbb{R}^d} d\boldsymbol{\xi} \int_{\mathbb{R}^d} d\mathbf{y} e^{-i\alpha \boldsymbol{\xi} \cdot (\mathbf{x} - \mathbf{y})} \mathcal{A}(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi}) \psi(\mathbf{y}) \\ &= \left(\frac{\alpha}{2\pi}\right)^d \int_{\mathbb{R}^d} d\mathbf{y} \int_{\mathbb{R}^d} d\boldsymbol{\xi} e^{-i\alpha \boldsymbol{\xi} \cdot (\mathbf{x} - \mathbf{y})} \mathcal{A}(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi}) \psi(\mathbf{y}). \end{aligned}$$

Proof. Let $\psi \in L^2(\mathbb{R}^d, \mathbb{C}^n)$ arbitrary. We first show that, applying the Fubini-Tonelli theorem and Hölder's inequality, the integrations may be interchanged, by estimating

$$\begin{aligned} &\int_{\mathbb{R}^d} d\boldsymbol{\xi} \int_{\mathbb{R}^d} d\mathbf{y} |e^{-i\alpha \boldsymbol{\xi} \cdot (\mathbf{x} - \mathbf{y})} \mathcal{A}(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi}) \psi(\mathbf{y})| \\ &\leq \int_{\mathbb{R}^d} d\boldsymbol{\xi} \sqrt{\int_{\mathbb{R}^d} d\mathbf{y} \|\mathcal{A}(\mathbf{x}, \mathbf{y}, \boldsymbol{\xi}) \psi(\mathbf{y})\|_{n \times n}^2} \|\psi\| < \infty. \end{aligned}$$

Next, we want to show that we can extend the integral representation to all $L^2(\mathbb{R}^d, \mathbb{C}^n)$ -functions, i.e that the above integral indeed corresponds to $(\text{Op}_\alpha(\mathcal{A}) \psi)(\mathbf{x})$. To this end let $(\psi_n)_{n \in \mathbb{N}}$ be a sequence of $C_0^\infty(\mathbb{R}^d, \mathbb{C}^n)$ -functions converging to ψ with respect to the $L^2(\mathbb{R}^d, \mathbb{C}^n)$ -norm. Then $\text{Op}_\alpha(\mathcal{A}) \psi$ is by definition given by

$$\text{Op}_\alpha(\mathcal{A}) \psi = \lim_{n \rightarrow \infty} \text{Op}_\alpha(\mathcal{A}) \psi_n, \quad (3.5)$$

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where the convergence is with respect to the $L^2(\mathbb{R}^d, \mathbb{C}^n)$ -norm. However, going over to a subsequence we can assume that this convergence also holds pointwise outside of a null set $N \subseteq \mathbb{R}^d$ (see for example [37, Theorem 3.12]). Moreover for any $\mathbf{x} \in \mathbb{R}^d \setminus N$ and we can compute

$$\begin{aligned} & \lim_{n \rightarrow \infty} \left| \left(\frac{\alpha}{2\pi} \right)^d \int_{\mathbb{R}^d} d\xi \int_{\mathbb{R}^d} d\mathbf{y} e^{-i\alpha\xi \cdot (\mathbf{x} - \mathbf{y})} \mathcal{A}(\mathbf{x}, \mathbf{y}, \xi) \psi(\mathbf{y}) - (\text{Op}_\alpha(\mathcal{A})\psi_n)(\mathbf{x}) \right| \\ &= \lim_{n \rightarrow \infty} \left| \left(\frac{\alpha}{2\pi} \right)^d \int_{\mathbb{R}^d} d\xi \int_{\mathbb{R}^d} d\mathbf{y} e^{-i\alpha\xi \cdot (\mathbf{x} - \mathbf{y})} \mathcal{A}(\mathbf{x}, \mathbf{y}, \xi) \Delta\psi_n(\mathbf{y}) \right| \\ &\leq \left(\frac{\alpha}{2\pi} \right)^d \int_{\mathbb{R}^d} d\xi \sqrt{\int_{\mathbb{R}^d} d\mathbf{y} \|\mathcal{A}(\mathbf{x}, \mathbf{y}, \xi)\|_{n \times n}^2} \lim_{n \rightarrow \infty} \|\Delta\psi_n\|^2 = 0, \end{aligned}$$

with $\Delta\psi_n := \psi - \psi_n$. Combining this estimate with the pointwise convergence (3.5) in $\mathbb{R}^d \setminus N$ yields the claim. \square

Remark 3.0.7. Let \mathcal{A} be a symbol such that for any $\mathbf{x} \in \mathbb{R}^d$ the function

$$\max_{\mathbf{y} \in \mathbb{R}^d} |\mathcal{A}(\mathbf{x}, \mathbf{y}, \cdot)| \in L^1(\mathbb{R}^d)$$

Then, the ξ - and \mathbf{y} -integrals in (2.8) are interchangeable for any $\psi \in L^1(\mathbb{R}^d, \mathbb{C}^n)$ by the Fubini-Tonelli theorem.

Note that this is in particular the case for symbols $\mathcal{A} \in L^1(\mathbb{R}^d, \mathbb{C}^{n \times n})$ which are independent of \mathbf{x} and \mathbf{y} . \diamond

Lemma 3.0.8. Let $\mathcal{A}(\mathbf{x}, \mathbf{y}, \xi) \equiv \mathcal{A}(\mathbf{x}, \xi)$ (i.e. \mathcal{A} is independent of \mathbf{y}) and $\mathcal{B}(\mathbf{x}, \mathbf{y}, \xi) \equiv \mathcal{B}(\mathbf{y}, \xi)$ be symbols such that $\text{Op}_\alpha(\mathcal{A})$ and $\text{Op}_\alpha(\mathcal{B})$ are well-defined and the following two conditions hold:

(i) The operator A defined for any $\psi \in L^2(\mathbb{R}^d, \mathbb{C}^n)$ by

$$(A\psi)(\mathbf{x}) := \int_{\mathbb{R}^n} e^{-i\xi\mathbf{x}} \mathcal{A}(\mathbf{x}, \xi/\alpha) \psi(\xi) d\xi,$$

is bounded on $L^2(\mathbb{R}^d, \mathbb{C}^n)$.

(ii) The operator B defined for any $\psi \in C_0^\infty(\mathbb{R}^d, \mathbb{C}^n)$ by

$$(B\psi)(\xi) := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^n} e^{i\xi\mathbf{y}} \mathcal{B}(\mathbf{y}, \xi/\alpha) \psi(\mathbf{y}) d\mathbf{y},$$

may be continuously extended to $L^2(\mathbb{R}^d, \mathbb{C}^n)$.

Then

$$\text{Op}_\alpha(\mathcal{A}) \text{Op}_\alpha(\mathcal{B}) = \text{Op}_\alpha(\mathcal{A}\mathcal{B}).$$

Proof. We first note that, due to condition (i),

$$\text{Op}_\alpha(\mathcal{A}) = A \mathcal{F}^{-1},$$

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as both sides define continuous operators on $L^2(\mathbb{R}^d, \mathbb{C}^n)$ and agree on the $C_0^\infty(\mathbb{R}^d, \mathbb{C}^n)$ -functions. Similarly, we conclude that

$$\text{Op}_\alpha(\mathcal{B}) = \mathcal{F} B .$$

This yields

$$\text{Op}_\alpha(\mathcal{A}) \text{Op}_\alpha(\mathcal{B}) = A B ,$$

and for any $\psi \in C_0^\infty(\mathbb{R}^d, \mathbb{C}^n)$ we have

$$\begin{aligned} (\text{Op}_\alpha(\mathcal{A})\text{Op}_\alpha(\mathcal{B})\psi)(\mathbf{x}) &= (AB\psi)(\mathbf{x}) \\ &= \frac{\alpha^d}{(2\pi)^d} \int_{\mathbb{R}^d} d\xi \int_{\mathbb{R}^n} d\mathbf{y} e^{-i\alpha\xi(\mathbf{x}-\mathbf{y})} \mathcal{A}(\mathbf{x}, \xi) \mathcal{B}(\mathbf{y}, \xi) \psi(\mathbf{y}) . \end{aligned}$$

Note that as $\text{Op}_\alpha(\mathcal{A})$ and $\text{Op}_\alpha(\mathcal{B})$ are bounded operators, so is $\text{Op}_\alpha(\mathcal{A}) \text{Op}_\alpha(\mathcal{B})$. This concludes the proof by continuous extension and by the definition of $\text{Op}_\alpha(\mathcal{AB})$. \square

Remark 3.0.9.

- (i) In what follows we often apply the previous Lemma in the case that \mathcal{B} is independent of both \mathbf{x} and \mathbf{y} and bounded by a constant $C > 0$. Then condition (ii) of Lemma 3.0.8 is obviously fulfilled, because for any $\psi \in C_0^\infty(\mathbb{R}^d, \mathbb{C}^n)$ we have

$$B\psi = \mathcal{B}(\cdot/\alpha) \mathcal{F}^{-1}\psi ,$$

and thus

$$\|B\psi\| = \|\mathcal{B}(\cdot/\alpha) \mathcal{F}^{-1}\psi\| \leq C \|\mathcal{F}^{-1}\psi\| = C \|\psi\| .$$

- (ii) Moreover, in the following, the symbol \mathcal{A} is sometimes also independent of both \mathbf{x} and \mathbf{y} and bounded by a constant $C > 0$ (with respect to the matrix sup-norm), then for any $\psi \in L^2(\mathbb{R}^d, \mathbb{C}^n)$ it follows that

$$A\psi = \mathcal{F} \mathcal{A}(\cdot/\alpha)\psi$$

and moreover

$$\|A\psi\| = \|\mathcal{F} \mathcal{A}(\cdot/\alpha)\psi\| = \|\mathcal{A}(\cdot/\alpha)\psi\| \leq C \|\psi\| .$$

Therefore, condition (i) in Lemma 3.0.8 is also fulfilled.

- (iii) Another case we will consider later is that $\mathcal{A} \equiv a$ is scalar-valued, independent of y and continuous with compact support

$$\text{supp } a \subseteq B_l(v) \times B_\delta(\zeta) .$$

Then from the following argument we conclude that A also fulfills condition (i) from Lemma 3.0.8. Take $\psi \in L^2(\mathbb{R}^d)$ arbitrary and consider

$$\begin{aligned} &\int |A\psi(x)|^2 dx \\ &= \int_{B_l(v)} dx \int_{B_\delta(\zeta)} d\xi \int_{B_\delta(\zeta)} d\xi' e^{-iu(\xi'-\xi)} \overline{\psi(\xi)} \psi(\xi') \overline{a(x, \xi/\alpha)} a(x, \xi'/\alpha) \end{aligned}$$

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Here we may interchange the order of integration due to the Fubini-Tonelli Theorem since

$$\begin{aligned} & \int_{B_l(v)} dx \int_{B_\delta(\zeta)} d\xi \int_{B_\delta(\zeta)} d\xi' \left| \overline{\psi(\xi)} \psi(\xi') \overline{a(x, \xi/\alpha)} a(x, \xi'/\alpha) \right| \\ & \leq C^2 \text{vol}(B_l(v)) \|\psi\|_{L^1(B_\delta(\zeta), \mathbb{C}^2)}^2 < \infty, \end{aligned}$$

where C is a bound for the absolute value of the continuous and compactly supported function a . Note that $L^2(B_\delta(\zeta), \mathbb{C}^2) \subseteq L^1(B_\delta(\zeta), \mathbb{C}^2)$ since $B_\delta(\zeta)$ is bounded. We then obtain

$$\begin{aligned} & \int |A\psi(u)|^2 du \\ & = \int d\xi \overline{\psi(\xi)} \int d\xi' \psi(\xi') \underbrace{\int dx e^{-ix(\xi' - \xi)} \overline{a(x, \xi/\alpha)} a(x, \xi'/\alpha)}_{=: \tilde{a}(\xi, \xi')} \\ & \leq \|\psi\| \int |\psi(\xi)| \|\tilde{a}(\xi, \cdot)\| d\xi \leq \|\psi\|^2 \sqrt{\int d\xi \int d\xi' |\tilde{a}(\xi, \xi')|^2}, \end{aligned}$$

where the function \tilde{a} is again continuous and compactly supported, which makes the last integral finite. We remark that in the last line we again applied Hölder's inequality twice.

This estimate shows that condition (i) from Lemma 3.0.8 is again satisfied. \diamond

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4.1. Further Preliminaries: The Dirac Propagator in the Schwarzschild Geometry

This section corresponds to [13, Section 2.3] (with some modifications).

4.1.1. The Integral Representation of the Propagator

We recall the form of the Dirac equation in the Schwarzschild geometry and its separation, closely following the presentation in [11] and [17]. Given a parameter $M > 0$ (the black hole mass), the exterior Schwarzschild metric reads

$$ds^2 = \sum_{j,k=0}^3 g_{jk} dx^j dx^k = \frac{\Delta(r)}{r^2} dt^2 - \frac{r^2}{\Delta(r)} dr^2 - r^2 d\vartheta^2 - r^2 \sin^2 \vartheta d\varphi^2,$$

where

$$\Delta(r) := r^2 - 2Mr.$$

Here the coordinates $(t, r, \vartheta, \varphi)$ take values in the intervals

$$-\infty < t < \infty, \quad r_1 < r < \infty, \quad 0 < \vartheta < \pi, \quad 0 < \varphi < 2\pi,$$

where $r_1 := 2M$ is the event horizon.

In this geometry, the Dirac operator takes the form (see also [17, Section 2.2]):

$$\mathcal{D} = \begin{pmatrix} 0 & 0 & \alpha_+ & \beta_+ \\ 0 & 0 & \beta_- & \alpha_- \\ \alpha_- & -\beta_+ & 0 & 0 \\ -\beta_- & \alpha_+ & 0 & 0 \end{pmatrix} \quad \text{with}$$

$$\beta_{\pm} = \frac{i}{r} \left(\frac{\partial}{\partial \vartheta} + \frac{\cot \vartheta}{2} \right) \pm \frac{1}{r \sin \vartheta} \frac{\partial}{\partial \varphi} \quad \text{and}$$

$$\alpha_{\pm} = -\frac{ir}{\sqrt{\Delta(r)}} \frac{\partial}{\partial t} \pm \frac{\sqrt{\Delta(r)}}{r} \left(i \frac{\partial}{\partial r} + i \frac{r-M}{2\Delta(r)} + \frac{i}{2r} \right).$$

It is most convenient to transform the radial coordinate to the so called *Regge-Wheeler-coordinate* $u \in \mathbb{R}$ defined by

$$u(r) = r + 2M \ln(r - 2M), \quad \text{so that} \quad \frac{du}{dr} = \frac{r^2}{\Delta(r)}.$$

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In this coordinate, the event horizon is located at $u \rightarrow -\infty$, whereas $u \rightarrow \infty$ corresponds to spatial infinity i.e. $r \rightarrow \infty$. Then the Dirac equation can be separated with the ansatz

$$\psi^{kn\omega}(t, u, \varphi, \vartheta) = e^{-ik\varphi} \frac{1}{\Delta(r)^{1/4} \sqrt{r}} \begin{pmatrix} X_-^{kn}(t, u) Y_-^{kn}(\vartheta) \\ X_+^{kn}(t, u) Y_+^{kn}(\vartheta) \\ X_+^{kn}(t, u) Y_-^{kn}(\vartheta) \\ X_-^{kn}(t, u) Y_+^{kn}(\vartheta) \end{pmatrix}$$

with $k \in \mathbb{Z} + 1/2$, $n \in \mathbb{N}$ and $\omega \in \mathbb{R}$. The angular functions Y_{\pm}^{kn} can be expressed in terms of spin-weighted spherical harmonics and form an orthonormal basis of $L^2((-1, 1), d\vartheta \cos \vartheta), \mathbb{C}^2$ (see [17, Section 2.4] with additional reference to [18]). The radial functions X_{\pm}^{kn} satisfy a system of partial differential equations

$$\begin{pmatrix} \sqrt{\Delta(r)} \mathcal{D}_+ & imr - \lambda \\ -imr - \lambda & \sqrt{\Delta(r)} \mathcal{D}_- \end{pmatrix} \begin{pmatrix} X_+^{kn} \\ X_-^{kn} \end{pmatrix} = 0, \quad (4.1)$$

where m denotes the particle mass and

$$\mathcal{D}_{\pm} = \frac{\partial}{\partial r} \mp \frac{r^2}{\Delta(r)} \frac{\partial}{\partial t},$$

for details see [11, Section 2]. Moreover, employing the ansatz

$$X_{\pm}^{kn}(t, u) = e^{-i\omega t} X_{\pm}^{kn\omega}(u),$$

equation (4.1) goes over to a system of ordinary differential equations, which admits two two-component fundamental solutions labeled by $a = 1, 2$. We denote the resulting Dirac solution by $X_a^{kn\omega} = (X_{a,+}^{kn\omega}, X_{a,-}^{kn\omega})$ (for more details on the choice of the fundamental solutions see Section 4.1.4 below).

As implied by [11, Theorem 3.6], one can then find the following formula for the mode-wise propagator:

Theorem 4.1.1. *Given initial radial data $X_0 \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$ at time $t = 0$, the corresponding solution $X \in C_{sc}^\infty(\mathbb{R}^2, \mathbb{C}^2)$ (i.e. smooth with spatially compact support) of the radial Dirac equation (4.1) can be written as*

$$X(t, u) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \sum_{a,b=1}^2 t_{ab}^{kn\omega} X_a^{kn\omega}(u) \langle X_b^{kn\omega} | X_0 \rangle,$$

for any $u, t \in \mathbb{R}$. The $X_a^{kn\omega}(u)$ are the fundamental solutions mentioned before. Here the coefficients $t_{ab}^{kn\omega}$ satisfy the relations

$$\overline{t_{ab}^{kn\omega}} = t_{ba}^{kn\omega},$$

and

$$\begin{cases} t_{ab}^{kn\omega} = \delta_{a,1} \delta_{b,1} & \text{if } |\omega| \leq m \\ t_{11}^{kn\omega} = t_{22} = \frac{1}{2}, \quad |t_{12}^{kn\omega}| \leq \frac{1}{2} & \text{if } |\omega| > m \end{cases}. \quad (4.2)$$

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4.1.2. Hamiltonian Formulation

We may rewrite the Dirac equation in Hamilton form, i.e.

$$\begin{aligned} i \frac{\partial}{\partial t} X^{kn}(t, u) &= (H_{kn} X^{kn}|_t)(u) \\ \iff (\mathcal{D} - m) e^{-ik\varphi} \frac{1}{\Delta(r)^{1/4} \sqrt{r}} \begin{pmatrix} X_-^{kn}(t, u) Y_-^{kn}(\vartheta) \\ X_+^{kn}(t, u) Y_+^{kn}(\vartheta) \\ X_+^{kn}(t, u) Y_-^{kn}(\vartheta) \\ X_-^{kn}(t, u) Y_+^{kn}(\vartheta) \end{pmatrix} &= 0, \end{aligned}$$

where the Hamiltonian H_{kn} is an essentially self-adjoint operator on $L^2(\mathbb{R}, \mathbb{C}^2)$ with dense domain $\mathcal{D}(H_{kn}) = \mathbf{C}_0^\infty(\mathbb{R}, \mathbb{C}^2)$. We identify it with its self-adjoint extension. This makes it possible to write the solution of the Cauchy problem as

$$X(t, u) = (e^{-itH_{kn}} X_0)(u) \quad \text{with } u \in \mathbb{R}.$$

Here, the initial data can be an arbitrary vector-valued function in the Hilbert space, i.e. $X_0 \in L^2(\mathbb{R}, \mathbb{C}^2)$. If we specialize to smooth initial data with compact support, i.e. $X_0 \in \mathbf{C}_0^\infty(\mathbb{R}, \mathbb{C}^2)$, then the time evolution operator can be written with the help of Theorem 4.1.1 as

$$(e^{-itH_{kn}} X_0)(u) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \sum_{a,b=1}^2 t_{ab}^{kn\omega} X_a^{kn\omega}(u) \langle X_b^{kn\omega} | X_0 \rangle, \\ \text{for } X_0 \in \mathbf{C}_0^\infty(\mathbb{R}, \mathbb{C}^2).$$

We point out that this formula does not immediately extend to general $X_0 \in L^2(\mathbb{R}, \mathbb{C}^2)$; we will come back to this technical issue a few times in this thesis.

4.1.3. Connection to the Full Propagator

In this section we explain, why it suffices to focus on one angular mode instead of the full propagator and why we can use the ordinary L^2 -scalar product instead of $(\cdot|\cdot)$.

To this end, we introduce the function

$$S := \Delta(r)^{1/4} \sqrt{r}.$$

Moreover, for each fixed $k \in \mathbb{Z} + 1/2$, $n \in \mathbb{Z}$ we denote by $(\mathcal{H}_0)_{kn}$ the completion of

$$V_{kn} := \text{span} \left\{ S^{-1} e^{-ik\varphi} \begin{pmatrix} X_-^{kn\omega}(u) Y_-^{kn}(\vartheta) \\ X_+^{kn\omega}(u) Y_+^{kn}(\vartheta) \\ X_+^{kn\omega}(u) Y_-^{kn}(\vartheta) \\ X_-^{kn\omega}(u) Y_+^{kn}(\vartheta) \end{pmatrix} \mid X = (X_+, X_-) \in L^2(\mathbb{R}, \mathbb{C}^2) \right\},$$

with respect to $(\cdot|\cdot)$, i.e.

$$(\mathcal{H}_0)_{kn} := \overline{V_{kn}}^{(\cdot|\cdot)}.$$

This space can be thought of as the mode-wise solution space of the Dirac-equation at time $t = 0$. Note that the entire Hilbert space of solutions at time $t = 0$, namely

$$\mathcal{H}|_{t=0} =: \mathcal{H}_0$$

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has the orthogonal decomposition

$$\mathcal{H}_0 = \bigoplus_{i \in \mathbb{N}} (\mathcal{H}_0)_{k_i n_i}. \quad (4.3)$$

(again with respect to $(\cdot|\cdot)$), where $((k_i, n_i))_{i \in \mathbb{N}}$ is an enumeration of $(\mathbb{Z} + 1/2) \times \mathbb{Z}$. Furthermore, each space $(\mathcal{H}_0)_{kn}$ can be connected with $L^2(\mathbb{R}, \mathbb{C}^2)$ using the mapping

$$\tilde{S} : ((\mathcal{H}_0)_{kn}, (\cdot|\cdot)) \rightarrow L^2(\mathbb{R}, \mathbb{C}^2),$$

which for any $(\psi_1, \dots, \psi_4) \in (\mathcal{H}_0)_{kn}$ is given by

$$\begin{aligned} & (\tilde{S}(\psi_1, \dots, \psi_4))_1 \\ &= \int_{-1}^1 d\vartheta \cos \vartheta \int_0^{2\pi} d\varphi \left\langle (\psi_2(u, \vartheta, \varphi), \psi_3(u, \vartheta, \varphi)) \left| e^{-ik\varphi} (Y_+^{kn}(\vartheta), Y_-^{kn}(\vartheta)) \right\rangle_{\mathbb{C}^2}, \\ & (\tilde{S}(\psi_1, \dots, \psi_4))_2 \\ &= \int_{-1}^1 d\vartheta \cos \vartheta \int_0^{2\pi} d\varphi \left\langle (\psi_4(u, \vartheta, \varphi), \psi_1(u, \vartheta, \varphi)) \left| e^{-ik\varphi} (Y_+^{kn}(\vartheta), Y_-^{kn}(\vartheta)) \right\rangle_{\mathbb{C}^2}. \end{aligned}$$

It has the inverse

$$\begin{aligned} \tilde{S}^{-1} : L^2(\mathbb{R}, \mathbb{C}^2) &\rightarrow ((\mathcal{H}_0)_{kn}, (\cdot|\cdot)), \\ (X_+, X_-) &\mapsto S^{-1} e^{-ik\varphi} \begin{pmatrix} X_-(u) Y_-^{kn}(\vartheta) \\ X_+(u) Y_+^{kn}(\vartheta) \\ X_+(u) Y_-^{kn}(\vartheta) \\ X_-(u) Y_+^{kn}(\vartheta) \end{pmatrix}, \end{aligned}$$

(where $\langle \cdot, \cdot \rangle_{\mathbb{C}^2}$ is the canonical scalar product on \mathbb{C}^2). Then a direct computation shows that the scalar products transform as

$$\langle \tilde{S}\psi | \tilde{S}\phi \rangle_{L^2} = (\psi | \phi) \quad \text{for any } \phi, \psi \in (\mathcal{H}_0)_{kn}.$$

This implies that \tilde{S} is unitary and we can identify the two spaces.

Now recall that the Dirac-equation can be separated by solutions of the form

$$\hat{\psi} = S^{-1} e^{-ik\varphi} \begin{pmatrix} X_-(t, u) Y_-^{kn}(\vartheta) \\ X_+(t, u) Y_+^{kn}(\vartheta) \\ X_+(t, u) Y_-^{kn}(\vartheta) \\ X_-(t, u) Y_+^{kn}(\vartheta) \end{pmatrix},$$

and can then be described mode-wise by the Hamiltonian H_{kn} on the space $L^2(\mathbb{R}, \mathbb{C}^2)$. Therefore denoting

$$\tilde{H}_{kn} := \tilde{S}^{-1} H_{kn} \tilde{S},$$

the diagonal block operator (with respect to the decomposition (4.3))

$$\tilde{H} := \text{diag}(\tilde{H}_{(k_1, n_1)}, \tilde{H}_{(k_2, n_2)}, \dots),$$

defines an essentially self-adjoint Hamiltonian for the original Dirac equation on the space \mathcal{H}_0 .

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Moreover, any function of \tilde{H} is of the same diagonal block operator form. The same holds for any multiplication operator by a characteristic function $\chi_{\tilde{U}}$, where \tilde{U} is a spherically symmetric set

$$\tilde{U} := U \times S^2 \subseteq \mathbb{R} \times S^2.$$

In particular, such an operator has the block operator representation

$$\chi_{\tilde{U}} = \text{diag}(\chi_{\tilde{U}}, \chi_{\tilde{U}}, \dots).$$

We therefore conclude that when computing traces of operators of the form

$$\chi_{\tilde{U}} f(\tilde{H}) \chi_{\tilde{U}} \quad \text{or} \quad f(\chi_{\tilde{U}} \tilde{H} \chi_{\tilde{U}}),$$

(for some suitable function f), we may consider each angular mode separately and then sum over the occupied states (and similarly for Schatten norms of such operators).

Moreover we point out that instead of $(\mathcal{H}_0)_{kn}$ we can work with the corresponding objects in $L^2(\mathbb{R}, \mathbb{C}^2)$, as the spaces are unitarily equivalent. Note, that then the multiplication operator $\chi_{\tilde{U}}$ goes over to the operator χ_U , i.e.

$$\tilde{S}^{-1} \chi_{\tilde{U}} \tilde{S} = \chi_U.$$

In particular this leads to

$$\text{tr} \left(\chi_{\tilde{U}} f(\tilde{H}) \chi_{\tilde{U}} \right) = \sum_{k,n} \text{tr} \left(\chi_{\tilde{U}} f(\tilde{H}_{kn}) \chi_{\tilde{U}} \right) = \sum_{k,n} \text{tr} \left(\chi_U f(H_{kn}) \chi_U \right)$$

and

$$\text{tr} f(\chi_{\tilde{U}} \tilde{H} \chi_{\tilde{U}}) = \sum_{k,n} \text{tr} f(\chi_{\tilde{U}} \tilde{H}_{kn} \chi_{\tilde{U}}) = \sum_{k,n} \text{tr} f(\chi_U H_{kn} \chi_U).$$

4.1.4. Asymptotics of the Radial Solutions

We now recall the asymptotics of the solutions of the radial ODEs and specify our choice of fundamental solutions. Since we want to consider the propagator at the horizon, we will need near-horizon approximations of the $X^{kn\omega}$'s. In order to control the resulting error terms, we now state a slightly stronger version of [11, Lemma 3.1], specialized to the Schwarzschild case.

Lemma 4.1.2. *For any $u_2 \in \mathbb{R}$ fixed, in Schwarzschild spacetime every solution $X(u, \omega) \equiv X^{kn\omega}(u)$ for $u \in (-\infty, u_2)$ is of the form*

$$X(u, \omega) = \begin{pmatrix} f_0^+ e^{-i\omega u} \\ f_0^- e^{i\omega u} \end{pmatrix} + R_0(u, \omega)$$

where the error term R_0 decays exponentially in u , uniformly in ω . More precisely, writing

$$R_0(u, \omega) = \begin{pmatrix} e^{-i\omega u} g^+(u, \omega) \\ e^{i\omega u} g^-(u, \omega) \end{pmatrix},$$

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the vector-valued function $g = (g^+, g^-)$ satisfies the bounds

$$|g(u, \omega)| \leq ce^{du}, \quad \left| \frac{d}{du} g(u, \omega) \right| \leq dce^{du} \quad \text{for all } u < u_2,$$

with coefficients $c, d > 0$ which can be chosen independently of ω and $u < u_2$ (only depending on M, m, k, n and u_2).

The proof, which follows the method in [11], is given in detail in Appendix A.

We can now explain how to construct the fundamental solutions $X_a = (X_a^+, X_a^-)$ for $a = 1$ and 2 (for this see also [11, Section 3] and [17, Section 2.4]). In the case that $|\omega| > m$ we choose X_1 and X_2 such that the corresponding functions f_0 from the previous lemma are of the form

$$f_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ for } X_1 \quad \text{and} \quad f_0 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \text{ for } X_2.$$

In the case $|\omega| \leq m$ we consider the behavior of solutions at infinity (i.e. asymptotically as $u \rightarrow \infty$). It turns out that there is (up to a prefactor) a unique fundamental solution which decays exponentially. We denote it by X_1 . Moreover, we choose X_2 as an exponentially increasing fundamental solution. We normalize the resulting fundamental system at the horizon by

$$\lim_{u \rightarrow -\infty} |X_{1/2}| = 1.$$

Representing these solutions in the form of the previous lemma we obtain

$$X_{1/2}(u) = \begin{pmatrix} e^{-i\omega u} f_{0,1/2}^+ \\ e^{i\omega u} f_{0,1/2}^- \end{pmatrix} + R_{0,1/2}(u)$$

with coefficients $f_{0,1/2}^\pm \in \mathbb{C}$. Due to the normalization, we know that

$$|f_{0,1/2}| = 1 \quad \text{and in particular} \quad |f_{0,1/2}^\pm| \leq 1.$$

Note however, that f_0 and R_0 from the previous Lemma may in general also depend on k and n , but we will suppress to corresponding indices for ease of notation.

4.2. The Regularized Projection Operator

This section corresponds to [13, Section 3] (with some modifications).

4.2.1. Definition and Basic Properties

As previously mentioned, the entropy is computed using the mode-wise regularized projection operator to the negative frequency space $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$. This operator emerges from $e^{-itH_{kn}}$ from Section 4.1.2 by setting $t = i\varepsilon$ (the “ $i\varepsilon$ ”-regularization) and restricting to the negative frequencies. So more precisely, for any $X \in \mathbf{C}_0^\infty(\mathbb{R}, \mathbb{C}^2)$ and $u \in \mathbb{R}$ the operator $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$ is defined by

$$((\Pi_{\text{BH}}^{(\varepsilon)})_{kn} X)(u) := \frac{1}{\pi} \int_{-\infty}^0 d\omega e^{\varepsilon\omega} \sum_{a,b=1}^2 t_{ab}^{kn\omega} X_a^{kn\omega}(u) \langle X_b^{kn\omega} | X \rangle. \quad (4.4)$$

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Moreover, we only consider finitely many occupied angular momentum modes. This can be thought of as an additional regularization, which we now make precise. Let $\mathcal{O} \subset (\mathbb{Z} + 1/2) \times \mathbb{N}$ be an arbitrary finite subset (the ‘‘occupied’’ modes). We then define the regularized projection operator to the negative frequency space $\Pi_{\text{BH}}^{(\varepsilon)}$ in the spirit of Section 4.1.3 as diagonal block operator

$$\begin{aligned} \Pi_{\text{BH}}^{(\varepsilon)} &:= \text{diag}((\check{\Pi}_{\text{BH}}^{(\varepsilon)})_{k_1 n_1}, (\check{\Pi}_{\text{BH}}^{(\varepsilon)})_{k_2 n_2}, \dots), \quad \text{with} \\ (\check{\Pi}_{\text{BH}}^{(\varepsilon)})_{kn} &:= \begin{cases} (\Pi_{\text{BH}}^{(\varepsilon)})_{kn}, & (k, n) \in \mathcal{O} \\ 0, & \text{else} \end{cases}, \end{aligned}$$

where again $((k_i, n_i))_{i \in \mathbb{N}}$ is an enumeration of $(\mathbb{Z} + 1/2) \times \mathbb{Z}$. Similar as explained in Section 4.1.3, for operators of this form it suffices to consider the corresponding operator for one angular mode $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$.

Since in this section we focus on one angular mode, we will drop the superscripts kn on the functions $X_a^{kn\omega}$ and $t_{ab}^{kn\omega}$ in (4.4). Moreover, we will sometimes write the ω -dependence of $X_a^{kn\omega}$ or $t_{ab}^{kn\omega}$ as an argument, i.e.

$$X_a^{kn\omega}(u) \equiv X_a^\omega(u) \equiv X_a(u, \omega) \quad \text{for any } u \in \mathbb{R}.$$

The asymptotics of the radial solutions at the horizon (Lemma 4.1.2) yield the following boundedness properties for the functions X_a^ω :

Remark 4.2.1. Given $u_2 \in \mathbb{R}$ and a constant $C > 0$, we consider functions $X, Z \in L^\infty(\mathbb{R}, \mathbb{C}^2)$ with the properties

$$\text{supp } X, \text{supp } Z \subset (-\infty, u_2] \quad \text{and} \quad \|X\|_{L^\infty}, \|Z\|_{L^\infty} < C.$$

Then the estimate in Lemma 4.1.2 yields

$$\sum_{a,b} |t_{ab}^\omega| |X(u)| |X_a^\omega(u, \omega)| |X_b^\omega(u', \omega)| |Z(u')| \leq 2C^2 (1 + ce^{du}) (1 + ce^{du'}),$$

for almost all $u, u', \omega \in \mathbb{R}$ and with constants c, d only depending on k, n and u_2 (as well as M and m).

If we assume in addition that X and Z are compactly supported, then for any $g \in L^1(\mathbb{R})$ the Lebesgue integral

$$\int_{-\infty}^{\infty} du \int_{-\infty}^{\infty} \frac{d\omega}{\pi} g(\omega) \int_{-\infty}^{\infty} du' t_{ab}^\omega X^\dagger(u) X_a^\omega(u, \omega) X_b^\omega(u', \omega)^\dagger Z(u'),$$

is well-defined. Moreover, applying Fubini we may interchange the order of integration arbitrarily. \diamond

Furthermore, we will need the following technical Lemma, which tells us that testing with smooth and compactly supported functions suffices to determine if a function is in L^2 and to estimate its L^2 -norm:

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Lemma 4.2.2. *Let N be a manifold with integration measure μ . Given a function $f \in L^1_{\text{loc}}(N, \mathbb{C}^n)$ (with $n \in \mathbb{N}$), we assume that the corresponding functional on the test functions*

$$\Phi : C_0^\infty(N, \mathbb{C}^n) \rightarrow \mathbb{C}, \quad v \mapsto \int_N \langle v(x) | f(x) \rangle_{\mathbb{C}^n} d\mu(x)$$

is bounded with respect to the L^2 -norm, i.e.

$$|\Phi(v)| \leq C \|v\|_{L^2(N, \mathbb{C}^n)} \quad \text{for all } v \in C_0^\infty(N, \mathbb{C}^n).$$

Then $f \in L^2(N, \mathbb{C}^n)$ and $\|f\|_{L^2(N, \mathbb{C}^n)} \leq C$.

Proof. Being bounded, the functional Φ can be extended continuously to $L^2(N, \mathbb{C}^n)$. The Fréchet-Riesz theorem makes it possible to represent this functional by an L^2 -function \hat{f} i.e. $\|\hat{f}\|_{L^2(N, \mathbb{C}^n)} \leq C$ and

$$\int_N \langle v(x), (f(x) - \hat{f}(x)) \rangle_{\mathbb{C}^n} d\mu(x) = 0 \quad \text{for all } v \in C_0^\infty(N, \mathbb{C}^n).$$

The fundamental lemma of the calculus of variations (for vector-valued functions on a manifold) yields that $f = \hat{f}$ almost everywhere. \square

Now we have all the tools to prove the boundedness of the operator $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$.

Lemma 4.2.3. *Equation (4.4) defines a continuous endomorphism $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$ on the space $L^2(\mathbb{R}, \mathbb{C}^2)$ with operator norm*

$$\|(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}\|_\infty \leq 1.$$

Proof. Let $X, Z \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$ be arbitrary. We apply $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$ to X and test with Z , i.e. consider

$$\left\langle Z \left| \frac{1}{\pi} \int_{-\infty}^0 d\omega e^{\varepsilon\omega} \sum_{a,b=1}^2 t_{ab}^\omega X_a(u, \omega) \langle X_b^\omega | X \rangle \right. \right\rangle =: (*).$$

Applying Remark 4.2.1, we may interchange integrations such that

$$(*) = \frac{1}{\pi} \int_{-\infty}^0 d\omega e^{\varepsilon\omega} \sum_{a,b=1}^2 t_{ab}^\omega \langle Z | X_a^\omega \rangle \langle X_b^\omega | X \rangle.$$

Moreover, from [11, proof of Theorem 3.6] we obtain the estimate

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \left| \sum_{a,b=1}^2 t_{ab}^\omega \langle X | X_a^\omega \rangle \langle X_b^\omega | Z \rangle \right| \leq \|X\| \|Z\|, \quad (4.5)$$

which yields

$$|(*)| \leq \|X\| \|Z\|.$$

Now by Lemma 4.2.2 we conclude that

$$(\Pi_{\text{BH}}^{(\varepsilon)})_{kn} X \in L^2(\mathbb{R}, \mathbb{C}^2) \quad \text{and} \quad \|(\Pi_{\text{BH}}^{(\varepsilon)})_{kn} X\| \leq \|X\|.$$

This estimate shows that $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$ extends to a continuous endomorphism on $L^2(\mathbb{R}, \mathbb{C}^2)$ with operator norm $\|(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}\|_\infty \leq 1$. \square

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4.2.2. Functional Calculus for H_{kn}

In order to derive some more properties of $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$ we need to employ the functional calculus of H_{kn} , as we want to rewrite

$$(\Pi_{\text{BH}}^{(\varepsilon)})_{kn} = g(H_{kn}),$$

for some suitable function g .

The following two Propositions constitute the main result of this section.

Proposition 4.2.4. *Let $g \in L^1(\mathbb{R})$ be a bounded real-valued function. Then for any $X \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$, the operator $g(H_{kn})$ has the integral representation*

$$(g(H_{kn})X)(u) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} g(\omega) \int_{-\infty}^{\infty} du' \sum_{a,b=1}^2 t_{ab}^\omega X_a(u, \omega) \langle X_b(u', \omega) | X(u') \rangle_{\mathbb{C}^2}, \quad (4.6)$$

valid for almost any $u \in \mathbb{R}$. Moreover, for any $Z \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$,

$$\langle Z | g(H_{kn})X \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} g(\omega) \sum_{a,b=1}^2 t_{ab}^\omega \langle Z | X_a^\omega \rangle \langle X_b^\omega | X \rangle, \quad (4.7)$$

Proposition 4.2.5. *Let $g \in L^1(\mathbb{R})$ be a bounded real-valued function. Then the operator $g(H_{kn})$ has the following properties:*

(i) $g(H_{kn})$ extends to a continuous endomorphism on $L^2(\mathbb{R}, \mathbb{C}^2)$ with operator norm

$$\|g(H_{kn})\|_\infty \leq \|g\|_{L^\infty(\mathbb{R})}.$$

(ii) The operator $g(H_{kn})$ is self-adjoint.

Note that the above proposition also follows from the spectral theorem for the (possibly unbounded) self-adjoint operator H_{kn} , however we give another proof later, using the integral representation which will follow from Proposition 4.2.4.

Proof of Proposition 4.2.4. We proceed in two steps.

First step: Proof for $g \in C_0^\infty(\mathbb{R})$: Since the Fourier transform is an automorphism on the Schwartz space, for any $g \in C_0^\infty(\mathbb{R})$ there is a function $\hat{g} \in S(\mathbb{R})$ such that

$$g(\omega) = \int \hat{g}(t) e^{-i\omega t} dt \quad \text{for any } \omega \in \mathbb{R}.$$

We evaluate the right hand side of (4.6) for $X \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$ arbitrary. Note that, when testing this with some $Z \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$, we may interchange the u - and ω -integrations due to an argument similar as in Remark 4.2.1 We thus obtain

$$\begin{aligned} & \left\langle Z \left| \frac{1}{\pi} \int g(\omega) \sum_{a,b=1}^2 t_{ab}(\omega) X_a^\omega \langle X_b^\omega | X \rangle d\omega \right. \right\rangle \\ &= \frac{1}{\pi} \int g(\omega) \sum_{a,b=1}^2 t_{ab}(\omega) \langle Z | X_a^\omega \rangle \langle X_b^\omega | X \rangle d\omega \\ &= \frac{1}{\pi} \int d\omega \left(\int dt \hat{g}(t) e^{-it\omega} \right) \sum_{a,b=1}^2 t_{ab}(\omega) \langle Z | X_a^\omega \rangle \langle X_b^\omega | X \rangle =: (*). \end{aligned}$$

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Using the rapid decay of \hat{g} together with (4.5), we can make use of the Fubini-Tonelli theorem which leads to

$$(*) = \frac{1}{\pi} \int dt \hat{g}(t) \int d\omega e^{-it\omega} \sum_{a,b=1}^2 t_{ab}(\omega) \langle Z | X_a^\omega \rangle \langle X_b^\omega | X \rangle .$$

It is shown in [11] that

$$(*) = \int \hat{g}(t) \langle Z | e^{-itH_{kn}} X \rangle dt .$$

Now we can again apply Fubini's theorem due to the rapid decay of \hat{g} and the boundedness of the operator $e^{-itH_{kn}}$ (which follows from 4.5), leading to

$$(*) = \langle Z | \left(\int \hat{g}(t) e^{-itH_{kn}} dt \right) X \rangle .$$

Next we use the multiplication operator version of the spectral theorem to rewrite H_{kn} as

$$H_{kn} = U f U^{-1} ,$$

with a suitable unitary operator U and a Borel function f on the corresponding measure space $(\sigma(H_{kn}), \Sigma, \mu)$. Then

$$e^{-itH_{kn}} = U e^{-itf} U^{-1} ,$$

and thus for any $\tilde{X} \in L^2(\mathbb{R}, \mathbb{C}^2)$ and almost any $x \in \sigma(H_{kn})$ it holds that

$$\left(\left(\int \hat{g}(t) e^{-itf} dt \right) U^{-1} \tilde{X} \right)(x) = \left(\int \hat{g}(t) e^{-itf(x)} dt \right) (U^{-1} \tilde{X})(x) = g(f(x)) (U^{-1} \tilde{X})(x) ,$$

which leads to

$$(*) = \langle Z | U(g \circ f) U^{-1} X \rangle = \langle Z | g(H_{kn}) X \rangle .$$

Thus we conclude that for any $X, Z \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$,

$$\left\langle Z \left| \frac{1}{\pi} \int_{-\infty}^{\infty} g(\omega) \sum_{a,b=1}^2 t_{ab}^\omega X_a^\omega \langle X_b^\omega | X \rangle \right. \right\rangle = \langle Z | g(H_{kn}) X \rangle .$$

Then Lemma 4.2.2 (together with similar estimates as before) yields that

$$\int_{-\infty}^{\infty} g(\omega) \sum_{a,b=1}^2 t_{ab}^\omega X_a^\omega(\cdot) \langle X_b^\omega | X \rangle \in L^2(\mathbb{R}, \mathbb{C}^2) ,$$

and therefore

$$g(H_{kn}) X = \sum_{kn} \int_{-\infty}^{\infty} g(\omega) \sum_{a,b=1}^2 t_{ab}^\omega X_a^\omega \langle X_b^\omega | X \rangle ,$$

almost everywhere.

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Second step: Proof for bounded $g \in L^1(\mathbb{R})$: We can find a sequence of test functions $(g_n)_{n \in \mathbb{N}}$ in $C_0^\infty(\mathbb{R})$ which is uniformly bounded by a constant $C > 0$ such that⁶

$$g_n \rightarrow g \quad \text{in } L^1(\mathbb{R}) \text{ and pointwise almost everywhere .}$$

Then with f and U as before (where we applied the spectral theorem to H_{kn}) we obtain for any $X \in L^2(\mathbb{R}, \mathbb{C}^2)$

$$g_n(f(x))(U^{-1}X)(x) \rightarrow g(f(x))(U^{-1}X)(x) \quad \text{for almost all } x \in \sigma(H_{kn}) .$$

Moreover, with the notation $\Delta g_n := g_n - g$ we can estimate

$$|\Delta g_n(f(x))(U^{-1}X)(x)| \leq (C + \|g\|_{L^\infty(\mathbb{R})}) |(U^{-1}X)(x)| \quad \text{for almost all } x \in \sigma(H_{kn}),$$

note that we can use $\|g\|_{L^\infty(\mathbb{R})}$ instead of $\|g\|_{L^\infty(\sigma(H_{kn}), \mu)}$, because g is bounded on all of \mathbb{R} . The previous estimate shows that the function $(C + \|g\|_{L^\infty(\mathbb{R})})|U^{-1}X| \in L^2(\sigma(H_{kn}), \mu)$ dominates the sequence of measurable functions $(\mathcal{M}_{\Delta g_n \circ f}(U^{-1}X))_{n \in \mathbb{N}}$ which additionally tends to zero pointwise almost everywhere. Therefore, making use of Lebesgue's dominated convergence theorem, we conclude that

$$\mathcal{M}_{g_n \circ f} U^{-1}X \rightarrow \mathcal{M}_{g \circ f} U^{-1}X \quad \text{in } L^2(\sigma(H_{kn}), \mu)$$

and thus

$$g_n(H_{kn})X \rightarrow g(H_{kn})X \quad \text{in } L^2(\mathbb{R}, \mathbb{C}^2) .$$

In particular, this implies that for any $X, Z \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$,

$$\langle Z | g_n(H_{kn})X \rangle \rightarrow \langle Z | g(H_{kn})X \rangle . \quad (4.8)$$

Next we need to show that the corresponding integral representations converge. To this end, we note that, just as in the first case, we may interchange integrations in the way

$$\begin{aligned} & \left\langle Z \left| \int_{-\infty}^{\infty} d\omega \Delta g_n(\omega) \sum_{a,b=1}^2 t_{ab}^\omega X_a^\omega \langle X_b^\omega | X \rangle \right. \right\rangle \\ &= \int_{-\infty}^{\infty} d\omega \Delta g_n(\omega) \sum_{a,b=1}^2 t_{ab}^\omega \langle Z | X_a^\omega \rangle \langle X_b^\omega | X \rangle =: (**). \end{aligned}$$

Now keep in mind that Remark 4.2.1 also yields the bound

$$\left| \sum_{a,b=1}^2 t_{ab}^\omega \langle Z | X_a^\omega \rangle \langle X_b^\omega | X \rangle \right| \leq C_{Z,X} ,$$

⁶Note that such a sequence can always be constructed from an arbitrary sequence $(\tilde{g}_n)_{n \in \mathbb{N}} \subseteq C_0^\infty(\mathbb{R})$ converging to g in $L^1(\mathbb{R})$ by smoothly cutting off the values of the function whenever its absolute value is larger than $\|g\|_{L^\infty(\mathbb{R})} + 1$ (to ensure uniform boundedness) and then going over to a subsequence (to get pointwise convergence a.e., see for example [37, Theorem 3.12]).

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which holds uniformly in ω . Using this inequality, we obtain the estimate

$$\begin{aligned} |(**)| &\leq \int_{-\infty}^{\infty} d\omega |\Delta g_n(\omega)| \left| \sum_{a,b=1}^2 t_{ab}^{\omega} \langle Z | X_a^{kn\omega} \rangle \langle X_b^{kn\omega} | X \rangle \right| \\ &\leq C_{Z,X} \int_{-\infty}^{\infty} |\Delta g_n(\omega)| d\omega \xrightarrow{n \rightarrow \infty} 0. \end{aligned}$$

Combined with (4.8), this finally yields for any $X, Z \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$

$$\langle Z | g(H_{kn})X \rangle = \left\langle Z \left| \sum_{kn} \int_{-\infty}^{\infty} d\omega g(\omega) \sum_{a,b=1}^2 t_{ab}^{\omega} X_a^{\omega} \langle X_b^{\omega} | X \rangle \right. \right\rangle.$$

We obtain (4.6) just as in the first case using Lemma 4.2.2. Finally, (4.7) follows by testing with Z and again interchanging the integrals as explained before. \square

Proof of Proposition 4.2.5.

(i) This follows directly from (4.7) together with (4.5), because

$$\begin{aligned} |\langle Z | g(H_{kn})X \rangle_{L^2}| &\stackrel{(4.7)}{=} \left| \int \frac{d\omega}{\pi} g(\omega) \sum_{a,b=1}^2 t_{ab}^{\omega} \langle Z | X_a^{\omega} \rangle \langle X_b^{\omega} | X \rangle \right| \\ &\stackrel{(4.5)}{\leq} \|g\|_{\infty} \|Z\| \|X\|. \end{aligned}$$

(ii) Using (4.6), the following computation shows that the operator $g(H_{kn})$ is self-adjoint because for any $X, Z \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$ we have

$$\begin{aligned} &\langle Z | g(H_{kn})X \rangle \\ &= \int du \int \frac{d\omega}{\pi} g(\omega) \int du' \sum_{a,b=1}^2 \overline{t_{ba}^{\omega} \langle X(u') | X_b(u', \omega) \rangle_{\mathbb{C}^2} \langle X_a(u, \omega) | Z(u) \rangle_{\mathbb{C}^2}} \\ &\stackrel{\text{Fubini}}{=} \int du' \int \frac{d\omega}{\pi} g(\omega) \int du \sum_{a,b=1}^2 t_{ab}^{\omega} \langle X(u') | X_a(u', \omega) \rangle_{\mathbb{C}^2} \langle X_b(u, \omega) | Z(u) \rangle_{\mathbb{C}^2} \\ &= \overline{\langle X | g(H_{kn})Z \rangle} = \langle g(H_{kn})Z | X \rangle, \end{aligned}$$

where in the second step we interchanged the names of the variables a and b . Note that applying Fubini is justified in view of Remark 4.2.1. From this equation the self-adjointness follows by continuous extension. \square

Now we apply these results to the operator $\Pi_{\text{BH}}^{(\varepsilon)}$:

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Corollary 4.2.6. *Consider the function*

$$g : \mathbb{R} \rightarrow \mathbb{R}, \quad \omega \mapsto \chi_{(-\infty, 0)}(\omega) e^{\varepsilon\omega},$$

then

$$(\Pi_{\text{BH}}^{(\varepsilon)})_{kn} = g(H_{kn}).$$

Moreover, for η_\varkappa as before we have:

$$\eta_\varkappa((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}) = (\eta_\varkappa \circ g)(H_{kn}). \quad (4.9)$$

Proof. First of all note that

$$(\Pi_{\text{BH}}^{(\varepsilon)})_{kn} = g(H_{kn}),$$

as both operators clearly agree on the dense subset $C_0^\infty(\mathbb{R}, \mathbb{C}^2) \subseteq L^2(\mathbb{R}, \mathbb{C}^2)$ (see Proposition 4.2.4) and are bounded (see Lemma 4.2.3 and Proposition 4.2.5). Equation (4.9) then follows by applying the functional calculus of H_{kn} (which is applicable due to Proposition 4.2.5). \square

4.2.3. Representation as a Pseudo-Differential Operator

The general idea is to rewrite $\Pi_{\text{BH}}^{(\varepsilon)}$ in the form of $\text{Op}_\alpha(\mathcal{A})$ and identify α with the inverse regularization constant.

With the help of (4.6), we obtain for any $\psi \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$

$$\begin{aligned} & ((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}\psi)(u) \\ &= \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} du' e^{-i\omega(u-u')} \left[\begin{pmatrix} \mathbf{a}_{\varepsilon,11}(\omega) & \mathbf{a}_{\varepsilon,12}(u, \omega) \\ \mathbf{a}_{\varepsilon,21}(u, \omega) & \mathbf{a}_{\varepsilon,22}(\omega) \end{pmatrix} \right. \\ & \quad \left. + \mathcal{R}_{0,\varepsilon}(u, u', \omega) \right] \psi(u'), \end{aligned} \quad (4.10)$$

with

$$\begin{aligned} \mathbf{a}_{\varepsilon,11}(\omega) &= e^{\varepsilon\omega} \left(|f_{0,1}^+(\omega)|^2 \chi_{(-m,0)}(\omega) + \frac{1}{2} \chi_{(-\infty,-m)}(\omega) \right) \\ \mathbf{a}_{\varepsilon,12}(u, \omega) &= e^{-\varepsilon\omega} e^{2i\omega u} \left(\overline{f_{0,1}^-(-\omega)} f_{0,1}^+(-\omega) \chi_{(0,m)}(\omega) + t_{12}(-\omega) \chi_{(m,\infty)}(\omega) \right) \\ \mathbf{a}_{\varepsilon,21}(u, \omega) &= e^{\varepsilon\omega} e^{2i\omega u} \left(f_{0,1}(\omega) \overline{f_{0,1}^+(\omega)} \chi_{(-m,0)}(\omega) + t_{21}(\omega) \chi_{(-\infty,-m)}(\omega) \right) \\ \mathbf{a}_{\varepsilon,22}(\omega) &= e^{-\varepsilon\omega} \left(|f_{0,1}^-(\omega)|^2 \chi_{(0,m)}(\omega) + \frac{1}{2} \chi_{(m,\infty)}(\omega) \right), \end{aligned}$$

and some error matrix $\mathcal{R}_{0,\varepsilon}(u, u', \omega)$ related to the error term $R_0(u, \omega)$ in Lemma 4.1.2. A more detailed computation is given in Appendix B. Moreover, a more precise form of $\mathcal{R}_{0,\varepsilon}(u, u', \omega)$ can be found in Section 4.5.1.

In order to bring $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$ in the form of $\text{Op}_\alpha(\mathcal{A})$, we need to rescale the ω -integral by a parameter α . As previously mentioned the idea in this chapter is to use ε^{-1} for the role of α . Introducing the notation

$$\xi := \varepsilon\omega,$$

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we thereby obtain for any $\psi \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$

$$\begin{aligned} & ((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}\psi)(u) \\ &= \frac{\varepsilon^{-1}}{\pi} \int_{-\infty}^{\infty} d\xi \int_{-\infty}^{\infty} du' e^{-i\xi(u-u')/\varepsilon} \left[\begin{pmatrix} \mathbf{a}_{\varepsilon,11}(\xi/\varepsilon) & \mathbf{a}_{\varepsilon,12}(u, \xi/\varepsilon) \\ \mathbf{a}_{\varepsilon,21}(u, \xi/\varepsilon) & \mathbf{a}_{\varepsilon,22}(\xi/\varepsilon) \end{pmatrix} \right. \\ & \quad \left. + \mathcal{R}_{0,\varepsilon}(u, u', \xi/\varepsilon) \right] \psi(u'), \end{aligned} \quad (4.11)$$

and set

$$\begin{aligned} \mathcal{R}_0^{(\varepsilon)}(u, u', \xi) &:= \mathcal{R}_{0,\varepsilon}(u, u', \xi/\varepsilon) \\ \mathcal{A}_{\text{BH}}^{(\varepsilon)}(u, \xi) &:= \begin{pmatrix} \mathbf{a}_{\varepsilon,11}(\xi/\varepsilon) & \mathbf{a}_{\varepsilon,12}(u, \xi/\varepsilon) \\ \mathbf{a}_{\varepsilon,21}(u, \xi/\varepsilon) & \mathbf{a}_{\varepsilon,22}(\xi/\varepsilon) \end{pmatrix}. \end{aligned} \quad (4.12)$$

Note that for the Schwarzschild case we always replace the arguments \mathbf{x} and \mathbf{y} in the definition of $\text{Op}_\alpha(\mathcal{A})$ by u and u' to emphasize that we are working with Regge-Wheeler coordinates.

4.3. Definition of the Entropy of the Horizon

This section corresponds to [13, Section 4] (with some modifications).

We now explain in more detail what we mean by the Rényi entanglement entropy of the horizon. Our starting point is the Rényi entropy operator from (1.2)

$$\eta_{\mathcal{K}}(\chi_{\tilde{\mathcal{K}}} \Pi_{\text{BH}}^{(\varepsilon)} \chi_{\tilde{\mathcal{K}}}) - \chi_{\tilde{\mathcal{K}}} \eta_{\mathcal{K}}(\Pi_{\text{BH}}^{(\varepsilon)}) \chi_{\tilde{\mathcal{K}}}, \quad (4.13)$$

where for the area we take an annular region $\tilde{\mathcal{K}}$ around the horizon of width ρ as defined in (1.3):

$$\tilde{\mathcal{K}} := (u_0 - \rho, u_0) \times S^2,$$

see also figure 4.1. Note that in the Regge-Wheeler coordinate u the horizon is located at $u \rightarrow -\infty$, so ultimately we want to consider the limit $u_0 \rightarrow -\infty$ and $\rho \rightarrow \infty$.

As explained in Section 4.1.3 we can compute the trace of the operator (4.13) mode wise going over to the subregions \mathcal{K} :

$$\begin{aligned} & \text{tr} \left(\eta_{\mathcal{K}}(\chi_{\tilde{\mathcal{K}}} \Pi_{\text{BH}}^{(\varepsilon)} \chi_{\tilde{\mathcal{K}}}) - \chi_{\tilde{\mathcal{K}}} \eta_{\mathcal{K}}(\Pi_{\text{BH}}^{(\varepsilon)}) \chi_{\tilde{\mathcal{K}}} \right) \\ &= \sum_{(k,n) \in \mathcal{O}} \text{tr} \left(\eta_{\mathcal{K}}(\chi_{\mathcal{K}} (\Pi_{\text{BH}}^{(\varepsilon)})_{kn} \chi_{\mathcal{K}}) - \chi_{\mathcal{K}} \eta_{\mathcal{K}}((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}) \chi_{\mathcal{K}} \right), \end{aligned}$$

where $\mathcal{O} \subset (\mathbb{Z} + 1/2) \times \mathbb{N}$ denotes the set of occupied modes as introduced in Section 4.2.1.

Thus we consider the mode-wise Rényi entropy of the black hole as defined in (1.5):

$$S_{\mathcal{K},kn}^{\text{BH}} = \frac{1}{2} \lim_{\rho \rightarrow \infty} \lim_{\varepsilon \searrow 0} \frac{1}{f(\varepsilon)} \lim_{u_0 \rightarrow -\infty} \text{tr} S_{\mathcal{K}}((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}, \mathcal{K})$$

where $f(\varepsilon)$ is a function describing the highest order of divergence in ε (we will later see that here $f(\varepsilon) = \ln(1/\varepsilon)$).

4. The Fermionic Entanglement Entropy of a Schwarzschild Black Hole

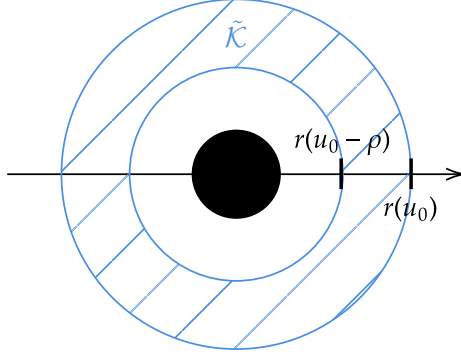


Figure 4.1.: Cross section visualizing the set $\tilde{\mathcal{K}} = \mathcal{K} \times S^2$ (similar to [13, Figure 2]).

The complete entanglement entropy of the black hole is then the sum over all occupied modes (see equation (1.6)).

In order to compute this in more detail, we will prove that

$$\lim_{\rho \rightarrow \infty} \lim_{\varepsilon \searrow 0} \frac{1}{f(\varepsilon)} \lim_{u_0 \rightarrow -\infty} \text{tr} \left(\eta_{\mathcal{K}}(\chi_{\mathcal{K}}(\Pi_{\text{BH}}^{(\varepsilon)})_{kn} \chi_{\mathcal{K}}) - \chi_{\mathcal{K}} \eta_{\mathcal{K}}((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}) \chi_{\mathcal{K}} \right) \quad (4.14)$$

$$= \lim_{\rho \rightarrow \infty} \lim_{\varepsilon \searrow 0} \frac{1}{f(\varepsilon)} \lim_{u_0 \rightarrow -\infty} \text{tr} \left(\eta_{\mathcal{K}}(\chi_{\mathcal{K}} \text{Op}_{1/\varepsilon}(\mathfrak{A}^{(0)}) \chi_{\mathcal{K}}) - \chi_{\mathcal{K}} \eta_{\mathcal{K}}(\text{Op}_{1/\varepsilon}(\mathfrak{A}^{(0)})) \chi_{\mathcal{K}} \right), \quad (4.15)$$

with the symbol

$$\mathfrak{A}^{(0)}(\xi) := \begin{pmatrix} e^{\xi} \chi_{(-\infty, 0)}(\xi) & 0 \\ 0 & e^{-\xi} \chi_{(0, \infty)}(\xi) \end{pmatrix}. \quad (4.16)$$

(We will later see that the operators in (4.14) and (4.15) are well-defined and trace class). The notation $\mathfrak{A}^{(0)}$ is supposed to emphasize the connection to the $\varepsilon \rightarrow 0$ limit of $\mathcal{A}_{\text{BH}}^{(\varepsilon)}$. Since $\mathfrak{A}^{(0)}$ is diagonal the computation of (4.15) is much easier than the one for (4.14). In fact we have

$$(4.15) = \sum_{j=1}^2 \lim_{\rho \rightarrow \infty} \lim_{\varepsilon \searrow \infty} \frac{1}{f(\varepsilon)} \lim_{u_0 \rightarrow -\infty} \text{tr} \left(\eta_{\mathcal{K}}(\chi_{\mathcal{K}} \text{Op}_{1/\varepsilon}(\mathfrak{a}_{0,j}) \chi_{\mathcal{K}}) - \chi_{\mathcal{K}} \eta_{\mathcal{K}}(\text{Op}_{1/\varepsilon}(\mathfrak{a}_{0,j})) \chi_{\mathcal{K}} \right)$$

with the scalar functions

$$\mathfrak{a}_{0,1}(\xi) := e^{\xi} \chi_{(-\infty, 0)}(\xi) \quad \text{and} \quad \mathfrak{a}_{0,2}(\xi) := e^{-\xi} \chi_{(0, \infty)}(\xi). \quad (4.17)$$

This reduces the computation of (4.15) to a problem for real-valued symbols for which many results are already established.

4.4. Trace of the Limiting Operator

This section corresponds to [13, Section 6] (with some modifications).

In this section we will only consider the operator $\text{Op}_{1/\varepsilon}(\mathfrak{a}_{0,1})$ in (4.17). Of course, the same methods apply to $\text{Op}_{1/\varepsilon}(\mathfrak{a}_{0,2})$.

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Remark 4.4.1. Note similar as in the proof of Lemma 3.0.1, the operator $\text{Op}_{1/\varepsilon}(\mathbf{a}_{0,1})$ can be rewritten as

$$\text{Op}_{1/\varepsilon}(\mathbf{a}_{0,1}) = \mathcal{F} \mathbf{a}_{0,1}(\varepsilon \cdot) \mathcal{F}^{-1},$$

and is therefore well-defined on all of $L^2(\mathbb{R})$. Moreover, due to Lemma 3.0.2 its integral representation extends to all Schwartz functions. Furthermore, if we add characteristic functions χ_U for some bounded subset $U \subseteq \mathbb{R}$, the integral representation of the operator $\chi_U \text{Op}_{1/\varepsilon}(\mathbf{a}_{0,1}) \chi_U$ holds on all of $L^2(\mathbb{R})$ due to Lemma 3.0.6. \diamond

4.4.1. A Theorem by Widom and Proof for Smooth Functions

The general idea is to make use of the following one-dimensional result by Widom in [49] (adapted to our notation).

Theorem 4.4.2. *Let $K, J \subseteq \mathbb{R}$ be intervals, $f \in C^\infty(\mathbb{R})$ a smooth function with $f(0) = 0$ and $a \in C^\infty(\mathbb{R}^2)$ a complex-valued Schwartz function which we identify with the symbol $a(x, y, \xi) \equiv a(x, \xi)$ for any $x, y, \xi \in \mathbb{R}$. Moreover, for any symbol b we denote its symmetric localization by*

$$A(b) := \frac{1}{2} \left(\chi_K \text{Op}_\alpha(I_J b) \chi_K + (\chi_K \text{Op}_\alpha(I_J b) \chi_K)^* \right), \quad (4.18)$$

(recall that I_J is the characteristic function corresponding to $J \subseteq \mathbb{R}$ with respect to the variable ξ). Then

$$\text{tr} \left(f(A(a)) - \chi_K \text{Op}_\alpha(I_J f(a)) \chi_K \right) = \frac{1}{4\pi^2} \ln(\alpha) \sum_i U(a(v_i); f) + \mathcal{O}(1),$$

where v_i are the vertices of $K \times J$ (see Figure 4.2) and

$$U(c; f) := \int_0^1 \frac{f(tc) - tf(c)}{t(1-t)} dt \quad \text{for any } c \in \mathbb{R}.$$

Remark 4.4.3. (i) To be precise, Widom considered operators with kernels

$$\frac{\alpha}{2\pi} \int dy \int d\xi e^{+i\alpha\xi(x-y)} a(x, \xi)$$

but the results can clearly be transferred using the transformation $\xi \rightarrow -\xi$.

(ii) Moreover, Widom considered operators of the form $\text{Op}_\alpha(a)$ whose integral representation extends to all of $L^2(K)$. We note that, in view of Lemma 3.0.6, this assumption holds for any operator $\text{Op}_\alpha(a)$ with Schwartz symbol $a = a(x, \xi)$, even if, a-priori, the integral representation holds only when inserting smooth compactly supported functions. \diamond

We want to apply the above theorem with

$$\alpha = \varepsilon^{-1}, \quad J = (-\infty, 0) =: \mathcal{J}, \quad K = \mathcal{K} = (u_0 - \rho, u_0),$$

where we choose f as a suitable approximation of the Rényi entropy function η_\varkappa (such that $f(0) = 0$) and a as an approximation of the diagonal matrix entries $\mathbf{a}_{0,j}$

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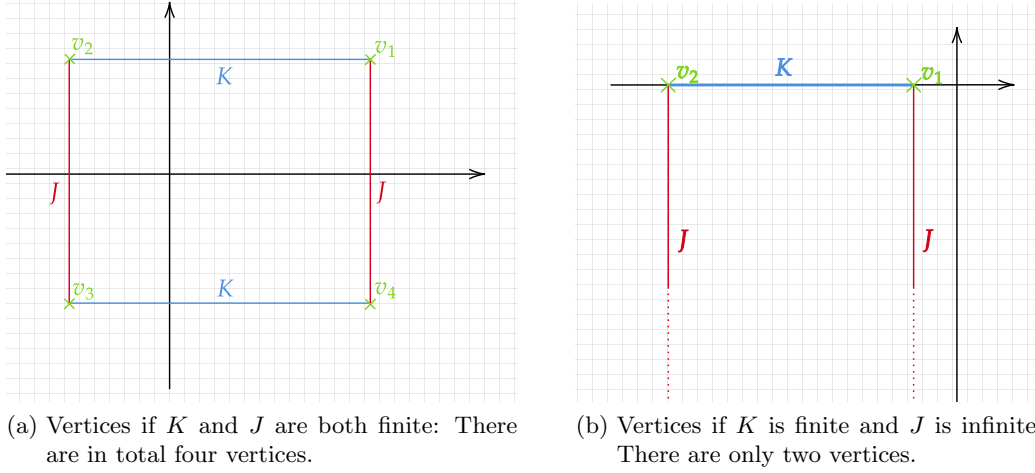


Figure 4.2.: Illustration with examples of the “vertices” in Theorem 4.4.2 (see [13, Figure 3]).

with $j = 1, 2$ in (4.17). For ease of notation, we only consider $a \approx \mathbf{a}_{0,1}$, noting that our methods apply similarly to $\mathbf{a}_{0,2}$. To be more precise, we first introduce the smooth non-negative cutoff functions $\Psi, \Phi \in C^\infty(\mathbb{R})$ with

$$\Psi(\xi) = \begin{cases} 1, & \xi \leq 0 \\ 0, & \xi > 1 \end{cases} \quad \text{and} \quad \Phi(u) = \begin{cases} 1, & u \in [-\rho, 0] \\ 0, & u \notin (-\rho - 1, 1), \end{cases}$$

and set $\Phi_{u_0}(x) := \Phi(x - u_0)$. Then we define

$$\mathbf{a}(u, \xi) := \Psi(\xi) \Phi_{u_0}(u) e^\xi, \quad (4.19)$$

this will play the role of a in Theorem 4.4.2. Note that then \mathbf{a} is a Schwartz function and

$$\chi_{\mathcal{K}} \text{Op}_{1/\varepsilon}(I_{\mathcal{J}} \mathbf{a}) \chi_{\mathcal{K}} = \chi_{\mathcal{K}} \text{Op}_{1/\varepsilon}(\mathbf{a}_{0,1}) \chi_{\mathcal{K}}.$$

Moreover, the resulting symbol clearly fulfills the condition of Lemma 3.0.6, so we can extend the corresponding integral representation to all $L^2(\mathbb{R}, \mathbb{C})$ -functions. In addition, the operator is self-adjoint, because of Lemma 3.0.1. This implies that we can leave out the symmetrization in (4.18), i.e.

$$A(\mathbf{a}) = \chi_{\mathcal{K}} \text{Op}_{1/\varepsilon}(I_{\mathcal{J}} \mathbf{a}) \chi_{\mathcal{K}} = \chi_{\mathcal{K}} \text{Op}_{1/\varepsilon}(\mathbf{a}_{0,1}) \chi_{\mathcal{K}}.$$

Furthermore, due to Lemma 3.0.1, we may pull out any function f as in the above Theorem 4.4.2 in the sense that

$$\chi_{\mathcal{K}} \text{Op}_{1/\varepsilon}(I_{\mathcal{J}} f(\mathbf{a})) \chi_{\mathcal{K}} = \chi_{\mathcal{K}} \text{Op}_{1/\varepsilon}(f(\mathbf{a}_{0,1})) \chi_{\mathcal{K}} = \chi_{\mathcal{K}} f(\text{Op}_{1/\varepsilon}(\mathbf{a}_{0,1})) \chi_{\mathcal{K}},$$

where we used that $\mathbf{a}_{0,1}$ vanishes outside \mathcal{J} and that $f(0) = 0$.

The vertices of $\mathcal{K} \times \mathcal{J}$ are (similar as in Figure 4.2 (B)) given by

$$v_1 = (u_0, 0) \quad \text{and} \quad v_2 = (u_0 - \rho, 0),$$

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and thus

$$\mathbf{a}(v_i) = 1, \quad \text{for any } i = 1, 2,$$

leading to

$$\begin{aligned} & \text{tr} \left(f(\chi_{\mathcal{K}} \text{Op}_{1/\varepsilon}(\mathbf{a}_{0,1}) \chi_{\mathcal{K}}) - \chi_{\mathcal{K}} f(\text{Op}_{1/\varepsilon}(\mathbf{a}_{0,1})) \chi_{\mathcal{K}} \right) \\ &= \frac{1}{2\pi^2} \ln(1/\varepsilon) U(1; f) + \mathcal{O}(1), \end{aligned} \quad (4.20)$$

valid for any $f \in C^\infty(\mathbb{R})$ with $f(0) = 0$.

Note that, using Lemma 3.0.3 and the fact that $\mathbf{a}_{0,1}$ does not depend on u or u' , the $\mathcal{O}(1)$ -term does not change when varying u_0 , and therefore the result stays same when we take the limit $u_0 \rightarrow -\infty$. We need to keep this in mind because we shall take the limit $u_0 \rightarrow -\infty$ before the limit $\varepsilon \searrow 0$ (see (1.5)).

4.4.2. Proof for Non-Differentiable Functions

Note that from now on we will use the scaling parameter α (which is simply a mathematical parameter) for more abstract results. In the end results we then apply this to $\alpha = 1/\varepsilon$ (with the regularization length ε), as in the following theorem, which constitutes the main result of this section.

Theorem 4.4.4. *Let $\mathcal{K} = (u_0 - \rho, u_0)$ (as in (1.4)) and $\mathbf{a}_{0,1}(\xi) = e^\xi \chi_{(-\infty, 0)}(\xi)$ as in (4.17). Moreover, let $g \in C^2(\mathbb{R} \setminus \{t_0, \dots, t_l\}) \cap C^0(\mathbb{R})$ satisfy Condition 2.2.5 with $g(0) = 0$. Then*

$$\lim_{\alpha \rightarrow \infty} \lim_{u_0 \rightarrow -\infty} \frac{1}{\ln \alpha} \text{tr} D_\alpha(g, \mathcal{K}, \mathbf{a}_{0,1}) = \frac{1}{2\pi^2} U(1; g).$$

In particular for $\alpha = 1/\varepsilon$,

$$\lim_{\varepsilon \searrow 0} \lim_{u_0 \rightarrow -\infty} \frac{1}{\ln(1/\varepsilon)} \text{tr} D_{1/\varepsilon}(g, \mathcal{K}, \mathbf{a}_{0,1}) = \frac{1}{2\pi^2} U(1; g). \quad (4.21)$$

In the proof of Theorem 4.4.4, we will apply Theorem 2.2.4 and Proposition 2.2.9. In order to complete the error estimates, we need to control the term $\|PA(\mathbb{1} - P)\|_{\sigma q}$ in the end. This can be done with the following lemma.

Lemma 4.4.5. *Let $u_0 \in \mathbb{R}$ arbitrary and $\mathcal{K} = (u_0 - \rho, u_0)$. Choose numbers $q \in (0, 1]$, $\alpha \geq 3$ and $\rho \geq 2$. Then the symbol $\mathbf{a}_{0,1}$ from (4.17) satisfies*

$$\|\chi_{\mathcal{K}} \text{Op}_\alpha(\mathbf{a}_{0,1}) (1 - \chi_{\mathcal{K}})\|_q^q \lesssim \ln \alpha.$$

with implicit constants independent of $\alpha \geq 3$ and u_0 .

Proof. First of all we make use Lemma 3.0.3 in order to replace the region \mathcal{K} by the interval $\mathcal{K}_0 := (-\rho, 0)$:

$$\|\chi_{\mathcal{K}} \text{Op}_\alpha(\mathbf{a}_{0,1}) (1 - \chi_{\mathcal{K}})\|_q^q = \|\chi_{\mathcal{K}_0} \text{Op}_\alpha(\mathbf{a}_{0,1}) (1 - \chi_{\mathcal{K}_0})\|_q^q.$$

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Next, let $(\Psi_j)_{j \in \mathbb{Z}}$ be a partition of unity with $\Psi_j(x) = \Psi_0(x - j)$ for all $j \in \mathbb{Z}$ and $\text{supp } \Psi_0 \subseteq (-\frac{1}{2}, \frac{3}{2})$. For any $j \in \mathbb{Z}$ we consider the symbols

$$\mathbf{a}_j(\xi) := \Psi_j(\xi) e^\xi,$$

Using the notation $\mathcal{J}_j := (j - 1, j)$ for any $j \in \mathbb{Z}_{\leq 0}$ we obtain with the help of Lemma 3.0.8 together with Remark 3.0.9,

$$\chi_{\mathcal{K}_0} \text{Op}_\alpha(I_{\mathcal{J}_j} \mathbf{a}_{0,1}) (1 - \chi_{\mathcal{K}_0}) = \chi_{\mathcal{K}_0} \text{Op}_\alpha(I_{\mathcal{J}_j} \mathbf{a}_j) (1 - \chi_{\mathcal{K}_0}) = \chi_{\mathcal{K}_0} P_{\mathcal{J}_j, \alpha} \text{Op}_\alpha(\mathbf{a}_j) (1 - \chi_{\mathcal{K}_0}),$$

so with the triangle inequality (2.4) we conclude that

$$\|\chi_{\mathcal{K}_0} \text{Op}_\alpha(\mathbf{a}_{0,1}) (1 - \chi_{\mathcal{K}_0})\|_q^q \leq \sum_{j \in \mathbb{Z}_{\leq 0}} \|\chi_{\mathcal{K}_0} P_{\mathcal{J}_j, \alpha} \text{Op}_\alpha(\mathbf{a}_j) (1 - \chi_{\mathcal{K}_0})\|_q^q. \quad (4.22)$$

In the next step we want to interchange $P_{\mathcal{J}_j, \alpha}$ and $\chi_{\mathcal{K}_0}$. To this end we make use of Lemma 2.2.11 giving

$$\|[P_{\mathcal{J}_j, \alpha}, \chi_{\mathcal{K}_0}]\|_q^q \leq 2\|(1 - \chi_{\mathcal{K}_0})P_{\mathcal{J}_j, \alpha}\chi_{\mathcal{K}_0}\|_q^q.$$

Moreover, using Remark 3.0.4 together with Corollary 2.2.14 we conclude that for any $j \in \mathbb{Z}_{\leq 0}$:

$$\|(1 - \chi_{\mathcal{K}_0})P_{\mathcal{J}_j, \alpha}\chi_{\mathcal{K}_0}\|_q^q = \|(1 - \chi_{\mathcal{K}_0})\text{Op}_\alpha(I_{\mathcal{J}_j})\chi_{\mathcal{K}_0}\|_q^q = \|(1 - \chi_{\mathcal{K}_0})\text{Op}_\alpha(I_{\mathcal{J}_0})\chi_{\mathcal{K}_0}\|_q^q \lesssim \ln \alpha,$$

with an implicit constant independent of $j \in \mathbb{Z}_{\leq 0}$, $\alpha \geq 2$ and u_0 . Moreover making use of Lemma 2.2.12 together with Lemma 3.0.2 and Remark 3.0.7 and the fact that

$$\mathbf{N}^{(1,1,2)}(\mathbf{a}_j; 1, 1) \lesssim e^j,$$

with an implicit constant independent of j we obtain for any $\alpha \geq 1$,

$$\|\text{Op}_\alpha(\mathbf{a}_j)\|_\infty^q \lesssim e^{qj},$$

again with an implicit constant independent of j and α . Using (2.5), this allows us to estimate

$$\begin{aligned} & \|\chi_{\mathcal{K}_0} P_{\mathcal{J}_j, \alpha} \text{Op}_\alpha(\mathbf{a}_j) (1 - \chi_{\mathcal{K}_0})\|_q^q \\ & \leq \|[\chi_{\mathcal{K}_0}, P_{\mathcal{J}_j, \alpha}] \text{Op}_\alpha(\mathbf{a}_j) (1 - \chi_{\mathcal{K}_0})\|_q^q + \|P_{\mathcal{J}_j, \alpha} \chi_{\mathcal{K}_0} \text{Op}_\alpha(\mathbf{a}_j) (1 - \chi_{\mathcal{K}_0})\|_q^q \\ & \leq \|[\chi_{\mathcal{K}_0}, P_{\mathcal{J}_j, \alpha}]\|_q^q \|\text{Op}_\alpha(\mathbf{a}_j) (1 - \chi_{\mathcal{K}_0})\|_\infty^q + \|P_{\mathcal{J}_j, \alpha}\|_\infty^q \|\chi_{\mathcal{K}_0} \text{Op}_\alpha(\mathbf{a}_j) (1 - \chi_{\mathcal{K}_0})\|_q^q \\ & \lesssim e^{qj} \ln \alpha + \|\chi_{\mathcal{K}_0} \text{Op}_\alpha(\mathbf{a}_j) (1 - \chi_{\mathcal{K}_0})\|_q^q, \end{aligned} \quad (4.23)$$

with an implicit constant independent of $j \in \mathbb{N}_0$ and $\alpha \geq 2$. Thus it remains to estimate the term $\|\chi_{\mathcal{K}_0} \text{Op}_\alpha(\mathbf{a}_j) (1 - \chi_{\mathcal{K}_0})\|_q^q$. To this end we want to apply Proposition 2.2.15 to \mathbf{a}_j . So choose $\delta = 2$ and $\zeta = j - 1/2$ and $k = \lfloor 2q^{-1} \rfloor + 1$, then

$$\mathbf{N}^{(k)}(\mathbf{a}_j; \delta) \lesssim e^j,$$

with an implicit constant independent of j . This yields

$$\|\chi_{\mathcal{K}_0} \text{Op}_\alpha(\mathbf{a}_j) (1 - \chi_{\mathcal{K}_0})\|_q^q \leq \|\chi_{\mathcal{K}_0} \text{Op}_\alpha(\mathbf{a}_j) (1 - \chi_{\mathcal{K}_0})\|_q^q \lesssim e^{qj}, \quad (4.24)$$

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with an implicit constant independent of j and $\alpha \geq 2$. Then, summarizing (4.22), (4.23) and (4.24) yields

$$\begin{aligned} \|\chi_{\mathcal{K}} \text{Op}_{\alpha}(\mathbf{a}_{0,1}) (1 - \chi_{\mathcal{K}})\|_q^q &\leq \sum_{j \in \mathbb{Z}_{\leq 0}} \|\chi_{\mathcal{K}_0} P_{\mathcal{J},\alpha} \text{Op}_{\alpha}(\mathbf{a}_j) (1 - \chi_{\mathcal{K}_0})\|_q^q \\ &\lesssim \sum_{j=0}^{\infty} e^{-qj} (\ln \alpha + 1) \lesssim \ln \alpha, \end{aligned}$$

with an implicit constant independent of $\alpha \geq 3$ and u_0 . \square

In the proof of Theorem 4.4.4 we will also make use of the following continuity result for $U(1; f)$.

Lemma 4.4.6. *Let f be a function on $[0, 1]$ with $f(0) = 0$.*

(i) *If $f \in \mathcal{C}^2([0, 1])$ denote*

$$\|f\|_{\mathcal{C}^2} := \max_{0 \leq k \leq 2} \max_{t \in [0,1]} |f^{(k)}(t)|.$$

Then,

$$|U(1; f)| \leq \frac{9}{2} \|f\|_{\mathcal{C}^2}.$$

(ii) *If f satisfies Condition 2.2.5 with $\mathbb{T} = \{z\}$ where $z = 0$ or $z = 1$ and is supported in $[z - R, z + R] \cap [0, 1]$ for some $R < \frac{1}{2}$, then*

$$|U(1; f)| \leq \|f\|_2 \frac{R^\gamma}{\gamma(1-R)}.$$

Proof. First split the integral in the definition of $U(1; f)$ as follows:

$$|U(1; f)| \leq \underbrace{\left| \int_0^{1/2} \frac{1}{t(1-t)} (f(t) - tf(1)) dt \right|}_{=:(I)} + \underbrace{\left| \int_{1/2}^1 \frac{1}{t(1-t)} (f(t) - tf(1)) dt \right|}_{=:(II)}.$$

(i) For the estimate of (I) consider the Taylor expansion for f around $t = 0$ keeping in mind that $f(0) = 0$:

$$f(t) = tf'(0) + \frac{t^2}{2} f''(\tilde{t}) \quad \text{for suitable } \tilde{t} \in [0, t],$$

and therefore

$$\begin{aligned} (I) &\leq \int_0^{1/2} \underbrace{\left| \frac{1}{(1-t)} \right|}_{\leq 2} \left(\underbrace{|f'(0)|}_{\leq \|f\|_{\mathcal{C}^2}} + \underbrace{\frac{|t/2|}{2}}_{\leq 1/4} \underbrace{|f''(\tilde{t})|}_{\leq \|f\|_{\mathcal{C}^2}} \right) dt + \int_0^{1/2} \underbrace{\left| \frac{1}{(1-t)} \right|}_{\leq 2} \underbrace{|f(1)|}_{\leq \|f\|_{\mathcal{C}^2}} dt \\ &\leq \frac{9}{4} \|f\|_{\mathcal{C}^2} \end{aligned}$$

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(note that \tilde{t} is actually a function of t , but this is unproblematic because f'' is uniformly bounded).

Similarly, for the estimate of (II) we use the Taylor expansion of f , but now around $t = 1$,

$$f(t) = f(1) + (t-1)f'(1) + \frac{(t-1)^2}{2}f''(\tilde{t}) \quad \text{for suitable } \tilde{t} \in [0, t].$$

We thus obtain

$$\begin{aligned} \text{(II)} &\leq \int_{1/2}^1 \left| \frac{1}{t(1-t)} \right| \left(|1-t| |f(1)| + |1-t| |f'(1)| + \frac{|1-t|^2}{2} |f''(\tilde{t})| \right) dt \\ &\leq \int_{1/2}^1 \underbrace{\left| \frac{1}{t} \right|}_{\leq 2} \left(\underbrace{|f(1)|}_{\leq \|f\|_{\mathcal{C}^2}} + \underbrace{|f'(1)|}_{\leq \|f\|_{\mathcal{C}^2}} + \underbrace{\frac{|1-t|}{2}}_{\leq 1/4} \underbrace{|f''(\tilde{t})|}_{\leq \|f\|_{\mathcal{C}^2}} \right) dt \leq \frac{9}{4} \|f\|_{\mathcal{C}^2}. \end{aligned}$$

(ii) (a) Case $z = 0$: First note that

$$|f(t)| \leq \|f\|_2 |t|^\gamma \quad \text{for any } t \in (0, 1/2).$$

This yields for $R < 1/2$,

$$\begin{aligned} |\text{(I)}| &= \left| \int_0^{1/2} \frac{1}{t(1-t)} f(t) dt \right| \leq \int_0^R \underbrace{\frac{1}{|1-t|}}_{\leq 1/(1-R)} \|f\|_2 |t|^{\gamma-1} dt \\ &\leq \frac{1}{1-R} \|f\|_2 \underbrace{\int_0^R |t|^{\gamma-1} dt}_{=R^\gamma/\gamma} \leq \|f\|_2 \frac{R^\gamma}{\gamma(1-R)}, \end{aligned}$$

Moreover, the integral (II) vanishes for $R < 1/2$.

(b) Case $z = 1$: Similarly as in the previous case, we now have

$$\text{(I)} = 0 \quad \text{for } R < 1/2.$$

Moreover, just as before, we can estimate

$$|f(t)| \leq \|f\|_2 |1-t|^\gamma \quad \text{for any } t \in (1/2, 1).$$

This yields for $R < 1/2$,

$$|\text{(ii)}| \leq \|f\|_2 \int_{1-R}^1 \frac{1}{|t|} |1-t|^{1-\gamma} dt \leq \|f\|_2 \frac{R^\gamma}{\gamma(1-R)}.$$

□

Now we have all the tools to prove Theorem 4.4.4.

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Proof of Theorem 4.4.4. Before beginning, we note that the u_0 -limit in (4.21) may be disregarded, because the symbol is translation invariant in position space (see Lemma 3.0.3, noting that $\mathbf{a}_{0,1}$ does not depend on $u \equiv \mathbf{x}$ or $u' \equiv \mathbf{y}$).

The remainder of the proof is based on the idea of [41, Proof of Theorem 4.4]. Let \mathbf{a} be the symbol in (4.19). By Lemma 2.2.12 together with Lemma 3.0.6, we can assume that the operator norm of $\text{Op}_\alpha(\mathbf{a})$ is uniformly bounded in α . Next, we want to apply Lemma 3.0.8 with $\mathcal{A} = \mathbf{a}$ and $\mathcal{B} = I_{\mathcal{J}}$ (recall that $\mathcal{J} = (-\infty, 0)$). In order to verify the conditions of this lemma, we first note that, Remark 3.0.9 (i) yields condition (ii), whereas condition (i) follows from the estimate

$$\begin{aligned} \int du \left| \int d\xi e^{-i\xi u} e^\xi \psi(\xi) \Psi(\xi) \Phi_{u_0}(u) \right|^2 &\leq \int_{u_0-\rho-1}^{u_0+1} du \left(\int d\xi \chi_{(-\infty,1)}(\xi) e^\xi |\psi(\xi)| \right)^2 \\ &\leq (\rho+2) \|\chi_{(-\infty,1)}\|_{L^2(\mathbb{R},\mathbb{C})}^2 \|\psi\|_{L^2(\mathbb{R},\mathbb{C})}^2, \end{aligned}$$

(which holds for any $\psi \in L^2(\mathbb{R})$). Now Lemma 3.0.8 yields

$$\text{Op}_\alpha(I_{\mathcal{J}} \mathbf{a}) = \text{Op}_\alpha(\mathbf{a}) P_{\alpha,\mathcal{J}}.$$

Since $P_{\alpha,\mathcal{J}}$ is a projection operator, we see that $\|\text{Op}_\alpha(I_{\mathcal{J}} \mathbf{a})\|_\infty \leq \|\text{Op}_\alpha(\mathbf{a})\|_\infty$ for all α . In particular, the operator $\text{Op}_\alpha(I_{\mathcal{J}} \mathbf{a})$ is bounded uniformly in α . Hence,

$$\|\chi_{\mathcal{K}} \text{Op}_\alpha(\mathbf{a}_{0,1}) \chi_{\mathcal{K}}\|_\infty = \|\chi_{\mathcal{K}} \text{Op}_\alpha(I_{\mathcal{J}} \mathbf{a}) \chi_{\mathcal{K}}\|_\infty \leq \|\text{Op}_\alpha(\mathbf{a})\|_\infty =: C_1,$$

uniformly in α . Moreover, the sup-norm of the symbol $\mathbf{a}_{0,1}$ itself is bounded by a constant C_2 . We conclude that we only need to consider the function g on the interval

$$[-\max\{C_1, C_2\}, \max\{C_1, C_2\}].$$

Therefore, we may assume that

$$\text{supp } g \subseteq [-C, C] \quad \text{with} \quad C := \max\{C_1, C_2\} + 1,$$

possibly replacing g by the function

$$\tilde{g} = \Psi_C g$$

with a smooth cutoff function $\Psi_C \geq 0$ such that

$$\Psi_C|_{[-C+1, C-1]} \equiv 1, \quad \text{and} \quad \text{supp } \Psi_C \subseteq [-C, C].$$

For ease of notation, we will write $g \equiv \tilde{g}$ in what follows.

We remark that the functions η_{\neq} which we plan to consider later already satisfy this property by definition with $C = 2$. From Proposition 2.2.9 and Lemma 4.4.5 we see that $D_\alpha(g, \mathcal{K}, \mathbf{a}_{0,1})$ is indeed trace class. We now compute this trace, proceeding in two steps.

First Step: Proof for $g \in \mathcal{C}^2(\mathbb{R})$.

To this end, we first apply the Weierstrass approximation theorem as given in [34, Theorem 1.6.2] to obtain a polynomial g_δ such that $f_\delta := g - g_\delta$ fulfills

$$\max_{0 \leq k \leq 2} \max_{|t| \leq C} |f_\delta^{(k)}(t)| \leq \delta. \quad (4.25)$$

4. The Fermionic Entanglement Entropy of a Schwarzschild Black Hole

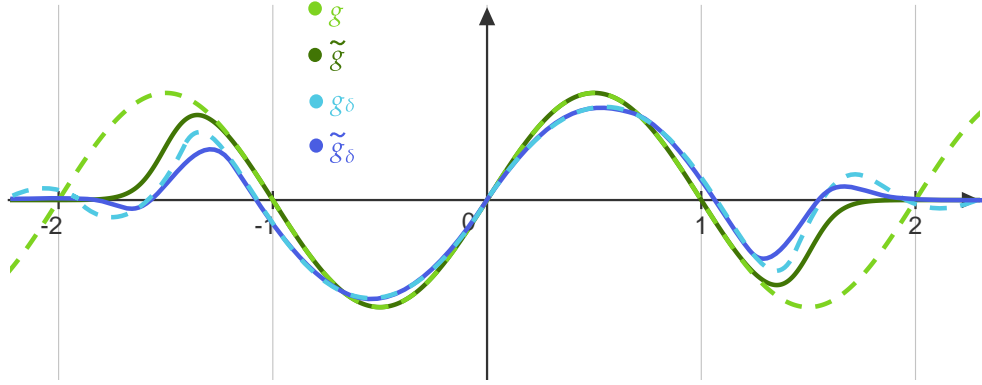


Figure 4.3.: Visualization of the cutoffs and approximations in the first step of the proof of Theorem 4.4.4 for $C = 2$. We start with a function g , which is first multiplied by the cutoff-function Ψ_C , giving \tilde{g} . This function is then approximated by a polynomial g_δ . Multiplying g_δ by the cutoff function Ψ_C results in a function which is here called \tilde{g}_δ (but does not directly appear in the proof). The function \tilde{f}_δ is then given by the difference between \tilde{g} and \tilde{g}_δ (see [13, Figure 5]).

Without loss of generality we can assume that $f_\delta(0) = 0$ (otherwise replace f_δ by the function $t \mapsto f_{\delta/2}(t) - f_{\delta/2}(0)$). In order to control the error of the polynomial approximation, we apply Theorem 2.2.4 with $k = 2$, $R = C$, some $\sigma \in (0, 1)$, $q = 1$ and

$$A = \text{Op}_\alpha(\mathbf{a}_{0,1}), \quad P = \chi\mathcal{K}, \quad g = \tilde{f}_\delta := f_\delta \Psi_C$$

(note that here g is the function in Theorem 2.2.4) where Ψ_C is the cutoff function from before (the cutoffs and approximation are visualized in Figure 4.3). This gives

$$\begin{aligned} & \|f_\delta(\chi\mathcal{K} \text{Op}_\alpha(\mathbf{a}_{0,1}) \chi\mathcal{K}) - \chi\mathcal{K} f_\delta(\text{Op}_\alpha(\mathbf{a}_{0,1})) \chi\mathcal{K}\|_1 \\ &= \|\tilde{f}_\delta(\chi\mathcal{K} \text{Op}_\alpha(\mathbf{a}_{0,1}) \chi\mathcal{K}) - \chi\mathcal{K} \tilde{f}_\delta(\text{Op}_\alpha(\mathbf{a}_{0,1})) \chi\mathcal{K}\|_1 \\ &\lesssim \delta \|\chi\mathcal{K} \text{Op}_\alpha(\mathbf{a}_{0,1}) (1 - \chi\mathcal{K})\|_\sigma^\sigma. \end{aligned}$$

with an implicit constant independent of δ and α . Moreover, applying Lemma 4.4.5, we conclude that for α large enough

$$\|f_\delta(\chi\mathcal{K} \text{Op}_\alpha(\mathbf{a}_{0,1}) \chi\mathcal{K}) - \chi\mathcal{K} f_\delta(\text{Op}_\alpha(\mathbf{a}_{0,1})) \chi\mathcal{K}\|_1 \lesssim \delta \ln \alpha,$$

(again with an implicit constant independent of δ and α). Using this inequality, we can estimate the trace by

$$\begin{aligned} \text{tr } D_\alpha(g, \mathcal{K}, \mathbf{a}_{0,1}) &\leq \text{tr } D_\alpha(g_\delta, \mathcal{K}, \mathbf{a}_{0,1}) + \|D_\alpha(f_\delta, \mathcal{K}, \mathbf{a}_{0,1})\|_1 \\ &\leq \text{tr } D_\alpha(g_\delta, \mathcal{K}, \mathbf{a}_{0,1}) + C_3 \delta \ln \alpha, \end{aligned}$$

with a constant C_3 independent of δ and α . In order to compute the remaining trace, we can again apply Theorem 4.4.2 (exactly as in the example (4.20)). This gives

$$\text{tr } D_\alpha(g_\delta, \mathcal{K}, \mathbf{a}_{0,1}) = \frac{1}{2\pi^2} \ln(\alpha) U(1; g_\delta) + \mathcal{O}(1),$$

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and thus

$$\mathrm{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) \leq \frac{1}{2\pi^2} \ln(\alpha) U(1; g_\delta) + C_3 \delta \ln \alpha + \mathcal{O}(1),$$

which yields,

$$\limsup_{\alpha \rightarrow \infty} \frac{1}{\ln \alpha} \mathrm{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) \leq \frac{1}{2\pi^2} U(1; g_\delta) + C_3 \delta. \quad (4.26)$$

Moreover, applying Lemma 4.4.6 (i) to f_δ we obtain due to (4.25)

$$\lim_{\delta \rightarrow 0} |U(1; g_\delta) - U(1; g)| = \lim_{\delta \rightarrow 0} |U(1; f_\delta)| = 0.$$

Therefore, taking the limit $\delta \rightarrow 0$ in (4.26) gives

$$\limsup_{\alpha \rightarrow \infty} \frac{1}{\ln \alpha} \mathrm{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) \leq \frac{1}{2\pi^2} U(1; g).$$

Analogously, using

$$\begin{aligned} \frac{1}{2\pi^2} \ln(\alpha) U(1; g_\delta) + \mathcal{O}(1) &= \mathrm{tr} D_\alpha(g_\delta, \mathcal{K}, \mathfrak{a}_{0,1}) \leq \mathrm{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) + \|D_\alpha(f_\delta, \mathcal{K}, \mathfrak{a}_{0,1})\|_1 \\ &\leq \mathrm{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) + C_3 \delta \ln \alpha, \end{aligned}$$

we obtain

$$\liminf_{\alpha \rightarrow \infty} \frac{1}{\ln \alpha} \mathrm{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) \geq \frac{1}{2\pi^2} U(1; g_\delta) + C_3 \delta.$$

Now we can take the limit $\delta \rightarrow 0$,

$$\liminf_{\alpha \rightarrow \infty} \frac{1}{\ln \alpha} \mathrm{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) \geq \frac{1}{2\pi^2} U(1; g).$$

Combining the inequalities for the lim sup and lim inf, we conclude that for any function $g \in \mathcal{C}^2(\mathbb{R})$,

$$\lim_{\alpha \rightarrow \infty} \frac{1}{\ln \alpha} \mathrm{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) = \frac{1}{2\pi^2} U(1; g). \quad (4.27)$$

Second Step: Proof for g as in claim.

By choosing a suitable partition of unity and making use of linearity, it suffices to consider the case $T = \{z\}$ meaning that g is non-differentiable only at one point z . Next we decompose g into two parts with a cutoff function $\xi \in \mathcal{C}_0^\infty(\mathbb{R})$ with the property that

$$\xi(t) = \begin{cases} 1, & |t| \leq 1/2 \\ 0, & |t| \geq 1 \end{cases}.$$

and writing

$$g = g_R^{(1)} + g_R^{(2)},$$

with

$$\begin{aligned} g_R^{(1)}(t) &:= g(t) \xi((t-z)/R) &\Rightarrow \mathrm{supp} g_R^{(1)} &\subseteq [z-R, z+R], \\ g_R^{(2)}(t) &:= g(t) - g_R^{(1)}(t) &\Rightarrow \mathrm{supp} g_R^{(2)} &\subseteq [-C, C]; \end{aligned}$$

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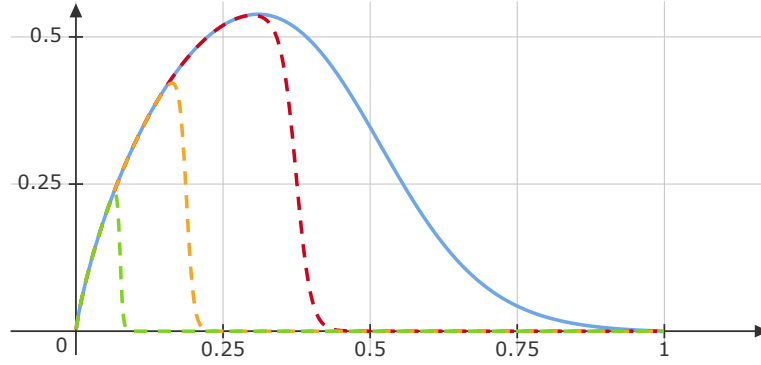


Figure 4.4.: Schematic plot of a function g (blue) with diverging derivative for $t \searrow 0$ with the corresponding functions $g_{1/2}^{(1)}$ (red), $g_{1/4}^{(1)}$ (orange) and $g_{1/10}^{(1)}$ (green): They are cutting out the non-differentiable point (see [13, Figure 6]).

see also Figure 4.4. Note that the derivatives of $g_R^{(1)}$ satisfy the bounds

$$\left(g_R^{(1)}\right)^{(k)}(t) = \sum_{n=0}^k c(n, k) g^{(k-n)}(t) \xi^{(n)}((t-z)/R) \frac{1}{R^n},$$

(with some numerical constants $c(n, k)$) and therefore the norm $\|\cdot\|_2$ in Condition 2.2.6 can be estimated by

$$\begin{aligned} \|g_R^{(1)}\|_2 &= \max_{0 \leq k \leq 2} \sup_{t \neq z} \left| \sum_{n=0}^k c(n, k) g^{(k-n)}(t) \xi^{(n)}((t-z)/R) \frac{1}{R^n} \right| \cdot |t-z|^{-\gamma+k} \\ &\leq \max_{0 \leq k \leq 2} \sup_{t \neq z} \sum_{n=0}^k |c(n, k)| |g^{(k-n)}(t)| |t-z|^{-\gamma+k-n} |\xi^{(n)}((t-z)/R)| \frac{|t-z|^n}{R^n}. \end{aligned}$$

Noting that on the support of $(g_R^{(1)})^{(k)}$ we have

$$\frac{|t-z|}{R} \leq 1,$$

we conclude that

$$\|g_R^{(1)}\|_2 \leq C_4 \|g\|_2 \quad (4.28)$$

with C_4 independent of R (also note that $\|g\|_2$ is bounded by assumption).

For what follows, it is also useful to keep in mind that

$$0 = g_R^{(1)}(0) = g_R^{(2)}(0).$$

Now we apply (4.27) to the function $g_R^{(2)}$ (which clearly is in $C^2(\mathbb{R})$),

$$\lim_{\alpha \rightarrow \infty} \frac{1}{\ln \alpha} \operatorname{tr} D_\alpha(g_R^{(2)}, \mathcal{K}, \mathfrak{a}_{0,1}) = U(1; g_R^{(2)}).$$

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Next, we apply Proposition 2.2.9 to $g_R^{(1)}$ with A and P as before, $q = 1$ and some $\sigma < \min\{1, \gamma\}$,

$$\|D_\alpha(g_R(1), \mathcal{K}, \mathfrak{a}_{0,1})\|_1 \leq C_\sigma \|g\|_2 R^{\gamma-\sigma} \|\chi_{\mathcal{K}} \text{Op}_\alpha(\mathfrak{a}_{0,1}) (1 - \chi_{\mathcal{K}})\|_\sigma^\sigma.$$

Then applying Lemma 4.4.5 (for α large enough) yields

$$\|D_\alpha(g_R(1), \mathcal{K}, \mathfrak{a}_{0,1})\|_1 \leq C_5 \|g\|_2 R^{\gamma-\sigma} \ln \alpha.$$

where the constant C_5 is independent of R and α . Just as before, it follows that

$$\begin{aligned} \limsup_{\alpha \rightarrow \infty} \frac{1}{\ln \alpha} \text{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) &\leq U(1; g_R^{(2)}) + C_5 \|g\|_2 R^{\gamma-\sigma}, \\ \liminf_{\alpha \rightarrow \infty} \frac{1}{\ln \alpha} \text{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) &\geq U(1; g_R^{(2)}) + C_5 \|g\|_2 R^{\gamma-\sigma}. \end{aligned}$$

The end result follows just as before by taking the limit $R \rightarrow 0$, provided that we can show the convergence $U(1; g_R^{(2)}) \rightarrow U(1; g)$ for $R \rightarrow 0$. To this end note that if $z \notin \{0, 1\}$ we have

$$|U(1; g_R^{(2)}) - U(1; g)| = |U(1; g_R^{(1)})| \leq C_6 R$$

for some $C_6 > 0$ independent of R provided that R is sufficiently small (more precisely, so small that $g_R^{(1)}$ vanishes in neighborhoods around 0 and 1; note that the integrand is supported in $[z - R, z + R]$ and bounded uniformly in R). These estimates show that $\lim_{R \rightarrow 0} U(1; g - g_R^{(2)}) = 0$ in the case that z is neither 0 nor 1. In the remaining cases where z is either 0 or 1 we can apply Lemma 4.4.6, which also yields due to (4.28),

$$\lim_{R \rightarrow 0} |U(1; g_R^{(2)}) - U(1; g)| = \lim_{R \rightarrow 0} |U(1; g_R^{(1)})| = C_4 \|g\|_2 \lim_{R \rightarrow 0} \frac{R^\gamma}{\gamma(1-R)} = 0.$$

This concludes the proof. \square

We finally apply Theorem 4.4.4 to the functions η_\varkappa and the matrix-valued symbol \mathfrak{A}^0 (see (1.1) and (4.16)).

Corollary 4.4.7. *For any $\varkappa > 0$, η_\varkappa , \mathcal{K} and $\mathfrak{A}^{(0)}$ as before,*

$$\lim_{\varepsilon \searrow 0} \lim_{u_0 \rightarrow \infty} \frac{1}{\ln(1/\varepsilon)} \text{tr} D_{1/\varepsilon}(\eta_\varkappa, \mathcal{K}, \mathfrak{A}^{(0)}) = \frac{1}{\pi^2} U(1; \eta_\varkappa) = \frac{1}{6} \frac{\varkappa + 1}{\varkappa}.$$

Moreover, in the case that $\varkappa = 1$, i.e. $\eta_\varkappa = \eta$, we can explicitly compute the coefficient $U(1; \eta)$ to give

$$\lim_{\varepsilon \searrow 0} \lim_{u_0 \rightarrow \infty} \frac{1}{\ln(1/\varepsilon)} \text{tr} D_{1/\varepsilon}(\eta, \mathcal{K}, \mathfrak{A}^{(0)}) = \frac{1}{\pi^2} U(1; \eta) = \frac{1}{3}.$$

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Proof. As explained in Example 2.2.8, the functions η_\varkappa satisfy Condition 2.2.5 with for any $\gamma < \min(1, \varkappa)$. Moreover, we have $\eta_\varkappa(0) = 0$ for any $\varkappa > 0$. Therefore we can apply Theorem 4.4.4 and obtain

$$\lim_{\varepsilon \searrow 0} \lim_{u_0 \rightarrow \infty} \frac{1}{\ln(1/\varepsilon)} \operatorname{tr} D_{1/\varepsilon}(\eta_\varkappa, \mathcal{K}, \mathfrak{a}_{0,1}) = \frac{1}{2\pi^2} U(1; \eta_\varkappa).$$

Repeating the procedure analogously for $\mathfrak{a}_{0,2}$ gives

$$\lim_{\varepsilon \searrow 0} \lim_{u_0 \rightarrow \infty} \frac{1}{\ln(1/\varepsilon)} \operatorname{tr} D_{1/\varepsilon}(\eta_\varkappa, \mathcal{K}, \mathfrak{a}_{0,2}) = \frac{1}{2\pi^2} U(1; \eta_\varkappa),$$

and therefore

$$\lim_{\varepsilon \searrow 0} \lim_{u_0 \rightarrow \infty} \frac{1}{\ln(1/\varepsilon)} \operatorname{tr} D_{1/\varepsilon}(\eta_\varkappa, \mathcal{K}, \mathfrak{Q}^{(0)}) = \frac{1}{\pi^2} U(1; \eta_\varkappa).$$

By [29, Appendix], evaluating $U(1; \eta_\varkappa)$ yields

$$U(1; \eta_\varkappa) = \int_0^1 \frac{\eta_\varkappa(t)}{t(1-t)} dt = \frac{\pi^2}{6} \frac{\varkappa + 1}{\varkappa},$$

and therefore

$$\lim_{\varepsilon \searrow 0} \lim_{u_0 \rightarrow \infty} \frac{1}{\ln(1/\varepsilon)} \operatorname{tr} D_{1/\varepsilon}(\eta_\varkappa, \mathcal{K}, \mathfrak{Q}^{(0)}) = \frac{1}{\pi^2} U(1; \eta_\varkappa) = \frac{1}{6} \frac{\varkappa + 1}{\varkappa}.$$

This concludes the proof. \square

Corollary 4.4.7 already looks quite similar to Theorem 1.0.1. The remaining task is to show equality in (4.15). To this end, we need to show that all the correction terms drop out in the limits $u_0 \rightarrow \infty$ and $\alpha \rightarrow \infty$. The next section is devoted to this task.

4.5. Estimating the Error Terms

This section corresponds to [13, Section 7] (with slight modifications).

In the previous section, we worked with the simplified kernel (4.16) and computed the corresponding entropy. In this section, we estimate all the errors, thereby proving the equality in (4.15). Our procedure is summarized as follows. Using (4.11), the regularized projection operator $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$ can be written as

$$(\Pi_{\text{BH}}^{(\varepsilon)})_{kn} = \text{Op}_{1/\varepsilon} \left(2 \left(\mathcal{A}_{\text{BH}}^{(\varepsilon)} + \mathcal{R}_0^{(\varepsilon)} \right) \right)$$

and $\mathcal{A}_{\text{BH}}^{(\varepsilon)}$ as in (4.12) and the error term

$$\mathcal{R}_0^{(\varepsilon)}(u, u', \xi) = \mathcal{R}_{0,\varepsilon}(u, u', \xi/\varepsilon),$$

We denote the corresponding symbol by

$$((\mathfrak{a}_{\text{full}})_{ij})_{1 \leq i, j \leq 2} := \mathcal{A}_{\text{full}}^{(\varepsilon)} := 2 \left(\mathcal{A}_{\text{BH}}^{(\varepsilon)} + \mathcal{R}_0^{(\varepsilon)} \right).$$

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In preparation, we translate \mathcal{K} to \mathcal{K}_0 with the help of the unitary operator T_{u_0} making use of Lemma 3.0.3 together with (3.4). Moreover, we use that the operators $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$ and $\text{Op}_{1/\varepsilon}(\mathfrak{A}^{(0)})$ are self-adjoint. We thus obtain

$$\begin{aligned} & D_{1/\varepsilon}(\eta_{\varkappa}, \mathcal{K}, \mathcal{A}_{\text{full}}^{(\varepsilon)}) - D_{1/\varepsilon}(\eta_{\varkappa}, \mathcal{K}, \mathfrak{A}^{(0)}) \\ &= D_{1/\varepsilon}(\eta_{\varkappa}, \mathcal{K}_0, T_{u_0}(\mathcal{A}_{\text{full}}^{(\varepsilon)})) - D_{1/\varepsilon}(\eta_{\varkappa}, \mathcal{K}_0, T_{u_0}(\mathfrak{A}^{(0)})), \end{aligned}$$

where $\mathfrak{A}^{(0)}$ is the kernel of the limiting operator from (4.16). Note that $T_{u_0}(\mathfrak{A}^{(0)}) = \mathfrak{A}^{(0)}$ since the symbol $\mathfrak{A}^{(0)}$ is independent of u and u' . Now we can estimate

$$\begin{aligned} & \|D_{1/\varepsilon}(\eta_{\varkappa}, \mathcal{K}_0, T_{u_0}(\mathcal{A}_{\text{full}}^{(\varepsilon)})) - D_{1/\varepsilon}(\eta_{\varkappa}, \mathcal{K}_0, \mathfrak{A}^{(0)})\|_1 \\ & \leq \left\| \eta_{\varkappa}(\chi_{\mathcal{K}_0} \text{Op}_{1/\varepsilon}(T_{u_0}(\mathcal{A}_{\text{full}}^{(\varepsilon)})) \chi_{\mathcal{K}_0}) - \eta_{\varkappa}(\chi_{\mathcal{K}_0} \text{Op}_{1/\varepsilon}(\mathfrak{A}^{(0)}) \chi_{\mathcal{K}_0}) \right\|_1 \quad (\text{I}) \\ & \quad + \left\| \chi_{\mathcal{K}_0} \left(\eta_{\varkappa}(\text{Op}_{1/\varepsilon}(T_{u_0}(\mathcal{A}_{\text{full}}^{(\varepsilon)}))) - \eta_{\varkappa}(\text{Op}_{1/\varepsilon}(\mathfrak{A}^{(0)})) \right) \chi_{\mathcal{K}_0} \right\|_1. \quad (\text{II}) \end{aligned}$$

In the following we will estimate the expressions (I) and (II) separately.

4.5.1. Estimate of the Error Term (I)

The following Theorem follows from [41, Theorem 2.4] (we use similar phrasing). It is related to Proposition 2.2.9.

Theorem 4.5.1. *Let \mathcal{H} be a Hilbert space and f a function which satisfies Condition 2.2.6 with some $\gamma, R > 0$. Let $\sigma \in (0, 1)$ with $\sigma < \gamma$. Let A, B be two bounded self-adjoint operators on \mathcal{H} . Suppose that $|A - B| \in \mathbf{S}_\sigma$, then*

$$\|f(A) - f(B)\|_1 \lesssim R^{\gamma-\sigma} \|f\|_2 \|A - B\|_\sigma^\sigma$$

with an implicit constant independent of A, B, f and R .

In order to apply this theorem to the functions η_{\varkappa} we use a partition of unity as explained in Remark 2.2.7. As explained in Example 2.2.8, we need to choose $\gamma < 1$ for $\varkappa = 1$ and $\gamma \leq \min\{\varkappa, 1\}$ otherwise. We will later see that with the methods in this thesis we can only estimate the error terms if $\varkappa > 2/3$. Thus we assume that $2/3 < \gamma < 1$ allowing us to treat all these cases simultaneously. This gives rise to the constraint

$$\sigma \in \left(\frac{2}{3}, 1 \right).$$

Setting $A = \chi_{\mathcal{K}_0} \text{Op}_{1/\varepsilon}(T_{u_0}(\mathcal{A}_{\text{full}}^{(\varepsilon)})) \chi_{\mathcal{K}_0}$ and $B = \chi_{\mathcal{K}_0} \text{Op}_{1/\varepsilon}(\mathfrak{A}^{(0)}) \chi_{\mathcal{K}_0}$ (which are clearly bounded and self-adjoint) by Theorem 4.5.1 we obtain

$$\begin{aligned} & \left\| \eta_{\varkappa}(\chi_{\mathcal{K}_0} \text{Op}_{1/\varepsilon}(T_{u_0}(\mathcal{A}_{\text{full}}^{(\varepsilon)})) \chi_{\mathcal{K}_0}) - \eta_{\varkappa}(\chi_{\mathcal{K}_0} \text{Op}_{1/\varepsilon}(\mathfrak{A}^{(0)}) \chi_{\mathcal{K}_0}) \right\|_1 \\ & \lesssim \left\| \chi_{\mathcal{K}_0} \text{Op}_{1/\varepsilon}(T_{u_0}(\mathcal{A}_{\text{full}}^{(\varepsilon)})) \chi_{\mathcal{K}_0} - \chi_{\mathcal{K}_0} \text{Op}_{1/\varepsilon}(\mathfrak{A}^{(0)}) \chi_{\mathcal{K}_0} \right\|_\sigma^\sigma \end{aligned}$$

with implicit constant independent of our choices of A and B (and thus in particular independent of u_0 and ε).

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For ease of notation, from now on we will denote

$$(\Delta(\mathbf{a}_{ij})_{u_0}^{(\varepsilon)})_{1 \leq i, j, \leq 2} := \Delta \mathcal{A}_{u_0}^{(\varepsilon)} := T_{u_0}(\mathcal{A}_{\text{full}}^{(\varepsilon)}) - \mathfrak{A}^{(0)}.$$

Note that the symbol $\Delta \mathcal{A}_{u_0}^{(\varepsilon)}$ is matrix-valued, but applying Remark 2.2.1 (ii), we obtain

$$\|\chi \mathcal{K}_0 \text{Op}_{1/\varepsilon}(\Delta \mathcal{A}_{u_0}^{(\varepsilon)}) \chi \mathcal{K}_0\|_{\sigma}^{\sigma} \leq \sum_{i, j=1}^2 \left\| \chi \mathcal{K}_0 \text{Op}_{1/\varepsilon}(\Delta(\mathbf{a}_{ij})_{u_0}^{(\varepsilon)}) \chi \mathcal{K}_0 \right\|_{\sigma}^{\sigma},$$

with the scalar-valued symbols $\Delta(\mathbf{a}_{ij})_{u_0}^{(\varepsilon)}$.

We now proceed by estimating the Schatten norms of the operators

$$\chi \mathcal{K}_0 \text{Op}_{1/\varepsilon}(\Delta(\mathbf{a}_{ij})_{u_0}^{(\varepsilon)}) \chi \mathcal{K}_0.$$

This will also show that these operators are well-defined and bounded on $L^2(\mathcal{K}_0, \mathbb{C})$. For the estimates we need the detailed form of the symbols given by

$$(\Delta \mathbf{a}_{11})_{u_0}^{(\varepsilon)}(u, u', \xi) = e^{\xi} \chi_{(-m\varepsilon, 0)}(\xi) \left(2|f_{0,1}^+|^2 \left(\frac{\xi}{\varepsilon} \right) - 1 \right) + r_{11} \left(u + u_0, u' + u_0, \frac{\xi}{\varepsilon} \right) \quad (4.29)$$

$$\begin{aligned} (\Delta \mathbf{a}_{12})_{u_0}^{(\varepsilon)}(u, u', \xi) &= 2e^{-\xi} e^{2i\xi(u+u_0)/\varepsilon} \left[\overline{f_{0,1}^-} \left(\frac{-\xi}{\varepsilon} \right) f_{0,1}^+ \left(\frac{-\xi}{\varepsilon} \right) \chi_{(0, m\varepsilon)}(\xi) \right. \\ &\quad \left. + t_{12} \left(\frac{-\xi}{\varepsilon} \right) \chi_{(m\varepsilon, \infty)}(\xi) \right] + r_{12} \left(u + u_0, u' + u_0, \frac{\xi}{\varepsilon} \right) \end{aligned} \quad (4.30)$$

$$\begin{aligned} (\Delta \mathbf{a}_{21})_{u_0}^{(\varepsilon)}(u, u', \xi) &= 2e^{\xi} e^{2i\xi(u+u_0)/\varepsilon} \left[f_{0,1}^- \left(\frac{\xi}{\varepsilon} \right) \overline{f_{0,1}^+} \left(\frac{\xi}{\varepsilon} \right) \chi_{(-m\varepsilon, 0)}(\xi) \right. \\ &\quad \left. + t_{21} \left(\frac{\xi}{\varepsilon} \right) \chi_{(-\infty, -m\varepsilon)}(\xi) \right] + r_{21} \left(u + u_0, u' + u_0, \frac{\xi}{\varepsilon} \right) \end{aligned} \quad (4.31)$$

$$\begin{aligned} (\Delta \mathbf{a}_{22})_{u_0}^{(\varepsilon)}(u, u', \xi) &= -e^{-\xi} \chi_{(0, m\varepsilon)}(\xi) \left(2|f_{0,1}^-|^2 \left(\frac{-\xi}{\varepsilon} \right) - 1 \right) \\ &\quad + r_{22} \left(u + u_0, u' + u_0, \frac{\xi}{\varepsilon} \right), \end{aligned} \quad (4.32)$$

with $r_{ij}(u, u', \xi) = (\mathcal{R}_{0,\varepsilon}(u, u', \xi))_{ij}$ for any $1 \leq i, j \leq 2$. Note that these equations only hold as long as u is smaller than some fixed u_2 which we may always assume as we take the limit $u_0 \rightarrow -\infty$.

One can group the terms in these functions into three classes, each of which will be estimated with different techniques: There are terms which are supported on “small” intervals $[-m\varepsilon/M, 0]$ or $[0, m\varepsilon/M]$. There are terms that contain the factor $e^{2Mi\xi(u+u_0)/\varepsilon}$, which makes them oscillate faster and faster as $u \leq u_0 \rightarrow -\infty$. And, finally, there are the r_{ij} -terms which decay rapidly in u and/or u' . Due to the triangle inequality (2.4), it will suffice to estimate each of these classes separately.

Error Terms with Small Support

We use this method for terms which do not depend on u and u' and which in ξ are supported in a small neighborhood of the origin. More precisely, these terms are of the form

$$\begin{aligned} e^{\xi} \chi_{(-m\varepsilon, 0)}(\xi) \left(2|f_{0,1}^+|^2 \left(\frac{\xi}{\varepsilon} \right) - 1 \right) &\quad \text{in } \Delta(\mathbf{a}_{11})_{u_0}^{(\varepsilon)} \\ -e^{-\xi} \chi_{(0, m\varepsilon)}(\xi) \left(2|f_{0,1}^-|^2 \left(\frac{-\xi}{\varepsilon} \right) - 1 \right) &\quad \text{in } \Delta(\mathbf{a}_{22})_{u_0}^{(\varepsilon)}. \end{aligned}$$

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Since these operators are translation invariant, we do not need to apply the translation operator T_{u_0} . This also shows that the error corresponding to these terms can be estimated independent of u_0 . For the estimate we will apply Proposition 2.2.13. As an example, consider

$$a^{(\varepsilon)}(\xi) := e^\xi \chi_{(-m\varepsilon, 0)}(\xi) \left(2|f_{0,1}^+|^2(\xi/\varepsilon) - 1 \right),$$

and

$$h := \chi_{\mathcal{K}},$$

which are both in $L_{\text{loc}}^2(\mathbb{R})$ because $|f_{0,1}^+|$ is bounded. Moreover, applying Lemma 3.0.5 (rescaling in momentum space) we obtain:

$$\text{Op}_{1/\varepsilon}(a^{(\varepsilon)}) = \text{Op}_1(a_\varepsilon),$$

for

$$a_\varepsilon(\xi) := a^{(\varepsilon)}(\varepsilon\xi) = e^{\varepsilon\xi} \chi_{(-m, 0)}(\xi) \left(2|f_{0,1}^+(\xi)|^2 - 1 \right),$$

which is again in $L_{\text{loc}}^2(\mathbb{R})$ for the same reasons as $a^{(\varepsilon)}$. Moreover, since $|f_{0,1}^+|$ is bounded, so is $a^{(\varepsilon)}$ and therefore by Lemma 3.0.2, the integral representation of $\text{Op}_\alpha(a^{(\varepsilon)})$ extends to all Schwartz functions for any $\alpha > 0$. Further, due to Remark 3.0.7 and the exponential decay of the symbol in ξ , the u' - and ξ -integrals in the integral representation are interchangeable for any Schwartz function.

Therefore we can now apply the estimate (2.5) together with Proposition 2.2.13 for $p \in (0, 1)$ arbitrary to obtain

$$\begin{aligned} \|\chi_{\mathcal{K}_0} \text{Op}_{1/\varepsilon}(a^{(\varepsilon)}) \chi_{\mathcal{K}_0}\|_p^p &\leq \|\chi_{\mathcal{K}_0}\|_\infty^p \|\chi_{\mathcal{K}_0} \text{Op}_{1/\varepsilon}(a^{(\varepsilon)})\|_p^p \leq \|\chi_{\mathcal{K}_0} \text{Op}_1(a_\varepsilon)\|_p^p \\ &\lesssim \|\chi_{\mathcal{K}_0}\|_{2,p}^p \|a_\varepsilon\|_{2,p}^p, \end{aligned}$$

with an implicit constant independent of ε . Next, noting that

$$\mathcal{K}_0 = (-\rho, 0) \subseteq (-[\rho], 0)$$

it follows that

$$\|\chi_{\mathcal{K}_0}\|_{2,p}^p \leq \sum_{-[\rho]}^0 1 = [\rho].$$

Similarly, since $|a_\varepsilon(\omega)|$ is bounded by one,

$$\|a_\varepsilon\|_{2,p}^p \leq \sum_{-[m]}^0 1 \leq [m].$$

Combining the last two inequalities, we conclude that

$$\|\chi_{\mathcal{K}_0} \text{Op}_{1/\varepsilon}(a^{(\varepsilon)}) \chi_{\mathcal{K}_0}\|_p^p \lesssim [\rho][m]. \quad (4.33)$$

Completely similar for

$$\tilde{a}^{(\varepsilon)}(\xi) := -e^{-\xi} \chi_{(0, m\varepsilon)}(\xi)$$

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we obtain

$$\|\chi_{\mathcal{K}_0} \text{Op}_{1/\varepsilon}(\tilde{a}^{(\varepsilon)}) \chi_{\mathcal{K}_0}\|_p^p \lesssim [\rho][m], \quad (4.34)$$

for any $p \in (0, 1)$ so in particular for $p = \sigma$. The estimates (4.33) and (4.34) show that the error terms with small support are independent of u_0 and bounded in ε . Therefore, dividing by $\ln(1/\varepsilon)$ and taking the limits $u_0 \rightarrow -\infty$ and $\varepsilon \searrow 0$ (in this order), these error terms drop out.

Rapidly Oscillating Error Terms

After translating the symbol by u_0 , these error terms are of the form

$$\begin{aligned} b^{(\varepsilon)}(u, \xi) &= e^{-\xi} e^{2i\xi(u+u_0)/\varepsilon} g(\xi/\varepsilon) \chi_{(0, \infty)}(\xi) \quad \text{or} \\ \tilde{b}^{(\varepsilon)}(u, \xi) &= e^{\xi} e^{2i\xi(u+u_0)/\varepsilon} \tilde{g}(\xi/\varepsilon) \chi_{(-\infty, 0)}(\xi), \end{aligned}$$

for some functions g, \tilde{g} which are measurable and bounded. They appear in $\Delta(\mathbf{a}_{12})_{u_0}^{(\varepsilon)}$ and $\Delta(\mathbf{a}_{21})_{u_0}^{(\varepsilon)}$. For simplicity, we restrict attention to the symbols of the form $b^{(\varepsilon)}$, but all estimates work for $\tilde{b}^{(\varepsilon)}$ in the same way. We make use of the result below, which follows from [7, Theorem 11.8.4 and Section 11.6.1] (we use similar phrasing).

Theorem 4.5.2. *Let $l \in \mathbb{N}_0$, $\mathcal{K}_0 = (-\rho, 0)$ and K be an integral operator on $L^2(\mathcal{K}_0)$ with kernel k , i.e. for any $\psi \in L^2(\mathcal{K}_0)$:*

$$(K\psi)(u) = \int_{\mathcal{K}_0} k(u, u') \psi(u') du'.$$

If $k(\cdot, u') \in W_2^l(\mathcal{K}_0)$ for almost all $u' \in \mathcal{K}_0$ with

$$\theta_2^2(t) := \int_{\mathcal{K}_0} \|k(\cdot, u')\|_{W_2^l(\mathcal{K}_0)}^2 du' < \infty,$$

then

$$K \in \mathbf{S}_p \quad \text{for } p > (1/2 + l)^{-1}$$

and

$$\|K\|_p \lesssim \theta_2(k),$$

with an implicit constant independent of k .

We want to apply this theorem for $p \in (0, 1)$ arbitrary, thus let $l \in \mathbb{N}$ arbitrary. Moreover, in view of Lemma 3.0.6, the integral representation corresponding to $\chi_{\mathcal{K}_0} \text{Op}_{1/\varepsilon}(b^{(\varepsilon)}) \chi_{\mathcal{K}_0}$ may be extended to all of $L^2(\mathbb{R})$ and we may interchange the $d\xi$ and du' integrations. Thus we need to estimate the norm θ_2 of the kernel of this operator. Therefore we consider kernels of the form

$$k_{u_0, \varepsilon}(u, u') := \frac{1}{2\pi\varepsilon} \int_0^\infty e^{-\xi} e^{i\xi(u+u'+u_0)/\varepsilon} g(\xi/\varepsilon) d\xi = \frac{1}{2\pi} \int_0^\infty e^{-\varepsilon\xi} e^{i\xi(u+u'+u_0)} g(\xi) d\xi,$$

where we used the change of variables $\xi \rightarrow \xi/\varepsilon$ (note that we could leave out the $\chi_{\mathcal{K}_0}$ -functions because in Theorem 4.5.2 we consider the operator on $L^2(\mathcal{K}_0)$). Since g

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is bounded and the factor $e^{-\varepsilon\xi}$ provides exponential decay, these kernels are always differentiable up to arbitrary orders with

$$\frac{d^s}{du^s} k_{u_0, \varepsilon}(u, u') = \frac{1}{2\pi} \int_0^\infty (i\xi)^s e^{-\varepsilon\xi} e^{i\xi(u+u'+u_0)} g(\xi) d\xi, \quad \text{for any } s \in \mathbb{N}.$$

Our goal is to show that the limit $u_0 \rightarrow -\infty$ of $\theta_2(k_{u_0, \varepsilon})$ is uniformly bounded in ε . To this end, we first note that for any $s \in \mathbb{N}_0$,

$$\frac{d^s}{du^s} k_{u_0, \varepsilon}(u, u') = \mathcal{F}(h_{s, (\varepsilon)})(-u - u' - u_0),$$

with

$$h_{s, \varepsilon}(\xi) := \frac{1}{\sqrt{2\pi}} (i\xi)^s e^{-\varepsilon\xi} g(\xi) \chi_{(0, \infty)}(\xi).$$

Now note that $h_{s, \varepsilon} \in L^1(\mathbb{R})$ for any $s \in \mathbb{N}_0$, so the Riemann-Lebesgue Lemma (see for example [8, Theorem 1]) tells us that for any $\delta > 0$ we can find $R = R(s, \varepsilon) > 0$ such that for any $l \in \mathbb{N}_0$,

$$\left| \frac{d^s}{du^s} k_{u_0, \varepsilon}(u, u') \right| \leq \delta \quad \text{for } |u + u' + u_0| > R.$$

Keeping in mind that for $u_0 \leq 0$,

$$|u + u' + u_0| \geq |u_0| \quad \text{for any } u, u' \in \mathcal{K}_0,$$

this is satisfied for $u_0 < -\max\{R(s, \varepsilon) \mid 0 \leq s \leq l\}$. This yields

$$\|k_{u_0, \varepsilon}(\cdot, y)\|_{W_2^l(\mathcal{K}_0)}^2 \leq l\delta^2\rho,$$

which in turn leads to

$$\theta_2(k_{u_0, \varepsilon}) \leq \sqrt{l}\delta\rho,$$

and so

$$\lim_{u_0 \rightarrow -\infty} \|\chi_{\mathcal{K}_0} \text{Op}_{1/\varepsilon}(b^{(\varepsilon)}) \chi_{\mathcal{K}_0}\|_p \lesssim \sqrt{l}\rho\delta,$$

for any $p \in (0, 1)$, so in particular this holds for $p = \sigma$. As δ is arbitrary, we conclude that the rapidly oscillating error terms vanish in the limit $u_0 \rightarrow -\infty$. We note for clarity that, since we take the limit $u_0 \rightarrow -\infty$ first, we do not need to worry about the dependence of the above estimate on ε .

Rapidly Decaying Error Terms

Finally, we consider the rapidly decaying error terms. In order to determine their detailed form, we first note that the solutions of the radial ODE have the asymptotics as given in Lemma 4.1.2 with an error term of the form

$$R_0(u) = \begin{pmatrix} e^{-i\omega u} R^+(u, \omega) \\ e^{-i\omega u} R^-(u, \omega) \end{pmatrix},$$

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with

$$R^\pm(u) := f^\pm(u) - f_0^\pm$$

and f^\pm as in (A.1). Using these asymptotics in the integral representation, the error terms in (4.29)–(4.32) can (similar as explained in Appendix B) be computed to be

$$\begin{aligned} r_{11}(u, u', \xi) &= \chi_{(-\infty, 0)}(\xi) e^{\varepsilon\xi} \sum_{a,b=1}^2 t_{ab}(\xi) \\ &\quad \times \left[f_{0,a}^+(\xi) \overline{R_b^+(u', \xi)} + R_a^+(u, \xi) \overline{f_{0,b}^+(\xi)} + R_a^+(u, \xi) \overline{R_b^+(u', \xi)} \right] \\ r_{12}(u, u', \xi) &= \chi_{(0, \infty)}(\xi) e^{2i\xi u} e^{-\varepsilon\xi} \sum_{a,b=1}^2 t_{ab}(-\xi) \\ &\quad \times \left[f_{0,a}^+(-\xi) \overline{R_b^-(u', -\xi)} + R_a^+(u, -\xi) \overline{f_{0,b}^+(-\xi)} + R_a^+(u, -\xi) \overline{R_b^-(u', -\xi)} \right] \\ r_{21}(u, u', \xi) &= \chi_{(-\infty, 0)}(\xi) e^{2i\xi u} e^{\varepsilon\xi} \sum_{a,b=1}^2 t_{ab}(\xi) \\ &\quad \times \left[f_{0,a}^-(\xi) \overline{R_b^+(u', \xi)} + R_a^-(u, \xi) \overline{f_{0,b}^+(\xi)} + R_a^-(u, \xi) \overline{R_b^+(u', \xi)} \right] \\ r_{22}(u, u', \xi) &= \chi_{(0, \infty)}(\xi) e^{-\varepsilon\xi} \sum_{a,b=1}^2 t_{ab}(-\xi) \\ &\quad \times \left[f_{0,a}^-(-\xi) \overline{R_b^-(u', -\xi)} + R_a^-(u, -\xi) \overline{f_{0,b}^-(-\xi)} + R_a^-(u, -\xi) \overline{R_b^-(u', -\xi)} \right]. \end{aligned}$$

Where by R_a^\pm we denote the function R^\pm corresponding to X_a for each $a = 1, 2$. In order to estimate these terms, the idea is to apply Theorem 4.5.2 (as well as the triangle inequality (2.4)) to each of these terms (with u and u' shifted by u_0) and then take the limit $u_0 \rightarrow -\infty$. We will do this for the first few terms explicitly, noting that the other terms can be estimated similarly.

Given u_2 , we know from Lemma 4.1.2 that for all $u < u_2$,

$$|R^\pm(u, \omega)| \leq ce^{du}, \quad |\partial_u R^\pm(u, \omega)| \leq cde^{du}, \quad (4.35)$$

with constants $c, d > 0$ that can be chosen independently of ω . Now for any $a, b \in \{1, 2\}$ we consider the symbol

$$c^{(\varepsilon)}(u, u', \xi) := \chi_{(-\infty, 0)}(\xi) e^\xi t_{ab}(\xi/\varepsilon) f_{0,a}^+(\xi/\varepsilon) \overline{R_b^+(u', \xi/\varepsilon)} \chi_{\mathcal{K}}(u) \chi_{\mathcal{K}}(u'),$$

which is contributing to $r_{11}(u, u', \xi/\varepsilon)$ (note that we again rescaled here in order to get the correct prefactor $e^{-i\xi(u-u')/\varepsilon}$). Translating by u_0 as before gives

$$\begin{aligned} \tilde{c}^{(\varepsilon)}(u, u', \xi) &= c^{(\varepsilon)}(u + u_0, u' + u_0, \xi) \\ &= \chi_{(-\infty, 0)}(\xi) e^\xi t_{ab}(\xi/\varepsilon) f_{0,a}^+(\xi/\varepsilon) \overline{R_b^+(u' + u_0, \xi/\varepsilon)} \chi_{\mathcal{K}_0}(u) \chi_{\mathcal{K}_0}(u'). \end{aligned}$$

By Lemma 3.0.6, the corresponding integral representation can be extended to all of $L^2(\mathcal{K}_0)$, since R^+ is bounded uniformly in ξ when restricted to the compact interval \mathcal{K}_0

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due to Lemma 4.1.2, and the e^ξ -factor provides exponential decay in ξ . Moreover, Lemma 3.0.6 again implies that we may interchange the $d\xi$ and du' integrations when restricting to \mathcal{K}_0 .

In order to estimate the corresponding error term, we apply Theorem 4.5.2 to the kernel

$$\tilde{k}_{u_0}^{(\varepsilon)}(u, u') := \frac{1}{2\pi} \int_{-\infty}^0 e^{-i\xi(u-u')} e^{\varepsilon\xi} t_{ab}(\xi) f_{0,a}^+(\xi) \overline{R_b^+(u' + u_0, \xi)} d\xi$$

(note that we rescaled back as before). This kernel is differentiable for similar reasons as before and

$$\frac{d}{du} \tilde{k}_{u_0, \varepsilon}(u, u') := \frac{1}{2\pi} \int_{-\infty}^0 (-i\xi) e^{-i\xi(u-u')} e^{\varepsilon\xi} t_{ab}(\xi) f_{0,a}^+(\xi) \overline{R_b^+(u' + u_0, \xi)} d\xi,$$

(note that we always normalize the solutions by $|f_0| = 1$). Using again the estimates for R^\pm in (4.35) yields for any $u, u' \in \mathcal{K}_0$:

$$\begin{aligned} |\tilde{k}_{u_0, \varepsilon}(u, u')| &\leq \frac{ce^{d(u'+u_0)}}{2\pi} \int_{-\infty}^0 e^{\varepsilon\xi} d\xi = \frac{ce^{d(u'+u_0)}}{2\pi\varepsilon}, \\ \left| \frac{d}{du} \tilde{k}_{u_0, \varepsilon}(u, u') \right| &\leq \frac{ce^{d(u'+u_0)}}{2\pi} \int_{-\infty}^0 |\xi| e^{\varepsilon\xi} d\xi = \frac{ce^{d(u'+u_0)}}{2\pi\varepsilon^2}, \end{aligned}$$

where we used that $|t_{ab}|, |f_{0,1/2}^\pm| \leq 1$. Therefore,

$$\|\tilde{k}_{u_0, \varepsilon}(\cdot, u')\|_{W_2^1(\mathcal{K}_0)}^2 = \rho \frac{c^2 e^{2d(u'+u_0)}}{4\pi^2 \varepsilon^4} (1 + \varepsilon^2),$$

and thus

$$\theta_2^2(\tilde{k}_{u_0, \varepsilon}) \leq C \frac{\rho^2}{\varepsilon^4} (1 + \varepsilon^2) e^{2du_0},$$

which makes clear that the corresponding error term vanishes in the limit $u_0 \rightarrow -\infty$.

We next consider a u -dependent contribution to r_{11} for some $a, b \in \{1, 2\}$ whose kernel is (by similar arguments as before) of the form

$$\check{k}_{u_0, \varepsilon}(u, u') := \frac{1}{2\pi} \int_{-\infty}^0 e^{-i\xi(u-u')} e^{\varepsilon\xi} t_{ab}(\xi) R_a^+(u + u_0, \xi) \overline{f_{0,b}^+(\xi)} d\xi.$$

Differentiating with respect to u gives

$$\begin{aligned} \frac{d}{du} \check{k}_{u_0, \varepsilon}(u, u') &:= \frac{1}{2\pi} \int_{-\infty}^0 e^{-i\xi(u-u')} e^{\varepsilon\xi} t_{ab}(\xi) \overline{f_{0,b}^+(\xi)} \\ &\quad \left(\partial_u R_a^+(u + u_0, \xi) - i\xi R_a^+(u + u_0, \xi) \right) d\xi, \end{aligned}$$

so that, similarly as before,

$$\begin{aligned} |\check{k}_{u_0, \varepsilon}(u, u')| &\leq \frac{ce^{d(u+u_0)}}{2\pi\varepsilon}, \\ \left| \frac{d}{du} \check{k}_{u_0, \varepsilon}(u, u') \right| &\leq \frac{c}{2\pi\varepsilon^2} e^{d(u+u_0)} (1 + \varepsilon). \end{aligned}$$

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This gives for $u < u_2 < 0$,

$$\|\check{k}_{u_0, \varepsilon}(\cdot, u')\|_{W_2^1(\mathcal{K}_0)}^2 \leq \rho C_\varepsilon e^{2du_0}$$

and thus

$$\theta_2(\check{k}_{u_0, \varepsilon})^2 \leq \rho^2 C_\varepsilon^2 e^{2du_0}$$

with a constant C_ε independent of u_0 . This shows that the corresponding error term again vanishes as $u_0 \rightarrow \infty$.

All the other error terms contributing to r_{ij} can be treated in the same way: The absolute value of the corresponding kernels (and their first derivatives) can always be estimated by a factor continuous in u and u' times a factor exponentially decaying in u_0 like e^{du_0} . This makes it possible to estimate θ_2 by a function which decays exponentially as $u_0 \rightarrow -\infty$.

Note that since we only have estimates for R^\pm and its first derivative in u , these estimates only apply for $\sigma \in (2/3, 1)$, i.e. $\varkappa \in (2/3, 1)$.

4.5.2. Estimate of the Error Term (II)

It remains to estimate the error terms (II) on page 56. First of all note that due to Lemma 3.0.3,

$$\begin{aligned} & \left\| \chi_{\mathcal{K}_0} \left(\eta_\varkappa(\text{Op}_{1/\varepsilon}(T_{u_0}(\mathcal{A}_{\text{full}}^{(\varepsilon)}))) - \eta_\varkappa(\text{Op}_{1/\varepsilon}(\mathfrak{A}^{(0)})) \right) \chi_{\mathcal{K}_0} \right\|_1 \\ &= \left\| \chi_{\mathcal{K}} \left(\eta_\varkappa((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}) - \eta_\varkappa(\text{Op}_{1/\varepsilon}(\mathfrak{A}^{(0)})) \right) \chi_{\mathcal{K}} \right\|_1 \end{aligned}$$

Luckily, in this case we can directly compute $\eta_\varkappa((\Pi_{\text{BH}}^{(\varepsilon)})_{kn})$ and $\eta_\varkappa(\text{Op}_{1/\varepsilon}(\mathfrak{A}^{(0)}))$, which simplifies the estimate. As explained before in Lemma 3.0.1 we have

$$\eta_\varkappa(\text{Op}_{1/\varepsilon}(\mathfrak{A}^{(0)})) = \text{Op}_{1/\varepsilon}(\eta_\varkappa(\mathfrak{A}^{(0)})).$$

Moreover, from Proposition 4.2.4 and Corollary 4.2.6 we conclude that for any function $X \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$,

$$\left(\eta_\varkappa((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}) X \right)(u) = \frac{1}{\pi} \int_{-\infty}^0 \eta_\varkappa(e^{\varepsilon\omega}) \sum_{a,b=1}^2 t_{ab}(\omega) X_a(u, \omega) \langle X_b(\cdot, \omega) | X \rangle d\omega.$$

Therefore we can rewrite

$$\eta_\varkappa(\text{Op}_{1/\varepsilon}(a_0)) - \eta_\varkappa((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}) = \text{Op}_{1/\varepsilon}(\Delta \tilde{\mathcal{A}}^{(\varepsilon)}), \quad (4.36)$$

where the entries of the symbol $\Delta \tilde{\mathcal{A}}^{(\varepsilon)} = (\Delta \tilde{\mathbf{a}}_{i,j}^{(\varepsilon)})_{1 \leq i, j \leq 2}$ are given by

$$\begin{aligned} \Delta \tilde{\mathbf{a}}_{1,1}^{(\varepsilon)}(u, u', \xi) &= \eta_\varkappa(e^\xi) e^{-\xi} (\Delta \mathbf{a}_{11})_0^{(\varepsilon)}(\xi), \\ \Delta \tilde{\mathbf{a}}_{1,2}^{(\varepsilon)}(u, u', \xi) &= \eta_\varkappa(e^{-\xi}) e^\xi (\Delta \mathbf{a}_{12})_0^{(\varepsilon)}(u, \xi), \\ \Delta \tilde{\mathbf{a}}_{2,1}^{(\varepsilon)}(u, u', \xi) &= \eta_\varkappa(e^\xi) e^{-\xi} (\Delta \mathbf{a}_{21})_0^{(\varepsilon)}(\xi), \\ \Delta \tilde{\mathbf{a}}_{2,2}^{(\varepsilon)}(u, u', \xi) &= \eta_\varkappa(e^{-\xi}) e^\xi (\Delta \mathbf{a}_{22})_0^{(\varepsilon)}(u, \xi), \end{aligned}$$

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note that $\text{Op}_{1/\varepsilon}(\Delta\tilde{\mathcal{A}}^{(\varepsilon)})$ is well defined, because the left hand side of (4.36) is a bounded operator which has the same integral representation on $\mathbb{C}_0^\infty(\mathbb{R}, \mathbb{C}^2)$. Thus these error terms are almost the same as before, except that the factor e^ξ has been replaced by $\eta_\varkappa(e^\xi)$ etc. and without translation by u_0 . Therefore, after applying Lemma 3.0.3 in order to again translate by u_0 ,

$$\left\| \chi\mathcal{K} \left(\eta_\varkappa \left(\left(\Pi_{\text{BH}}^{(\varepsilon)} \right)_{kn} \right) - \eta_\varkappa \left(\text{Op}_\alpha(\mathfrak{A}^{(0)}) \right) \right) \chi\mathcal{K} \right\|_1 = \left\| \chi\mathcal{K}_0 \text{Op}_\alpha(T_{u_0}(\Delta\tilde{\mathcal{A}}^{(\varepsilon)})) \chi\mathcal{K}_0 \right\|_1,$$

we can use the same techniques as before since the functions $\eta_\varkappa(e^{\varepsilon\xi})$ have similar decay-properties for $\xi \rightarrow -\infty$ and $\xi \nearrow 0$ as $e^{\varepsilon\xi}$, as the following lemma shows.

Lemma 4.5.3. *Let $\varkappa, a > 0$ arbitrary and denote $\tilde{\varkappa} := \min\{\varkappa, 1\}$, then*

$$\chi_{(-\infty, 0)}(\xi) \eta_\varkappa(e^{a\xi}) \simeq \chi_{(-\infty, 0)}(\xi) e^{\tilde{\varkappa} a \xi} \quad (4.37)$$

$$\lim_{\xi \nearrow 0} \eta_\varkappa(e^{a\xi}) = 0 \quad (4.38)$$

By symmetry reasons this also implies corresponding decay properties for $\eta_\varkappa(e^{-\xi})$ for $\xi \rightarrow \infty$ and $\xi \searrow 0$.

Proof of Lemma 4.5.3. We start with the case that $\varkappa = 1$ and first rewrite these functions in more detail as

$$\eta(e^{a\xi}) = -a\xi e^{a\xi} - (1 - e^{-a\xi}) \ln(1 - e^{a\xi}).$$

The term $-a\xi e^{a\xi}$ clearly satisfies the claim. Moreover,

$$\begin{aligned} \lim_{\xi \nearrow 0} \left((1 - e^{a\xi}) \ln(1 - e^{a\xi}) \right) &= \lim_{\xi \nearrow 0} \frac{\ln(1 - e^{a\xi})}{(1 - e^{a\xi})^{-1}} \stackrel{L'H}{=} \lim_{\xi \nearrow 0} \frac{-a(1 - e^{a\xi})^{-1} e^{a\xi}}{a(1 - e^{a\xi})^{-2} e^{a\xi}} \\ &= - \lim_{\xi \nearrow 0} (1 - e^{a\xi}) = 0, \end{aligned}$$

(where “L’H” denotes the use of L’Hôpital’s rule) showing that these terms are bounded near $\xi = 0$. Next,

$$\lim_{\xi \rightarrow -\infty} \frac{\ln(1 - e^{a\xi})}{e^{a\xi}} \stackrel{L'H}{=} \lim_{\xi \rightarrow -\infty} \frac{-a(1 - e^{a\xi})^{-1} e^{a\xi}}{a e^{a\xi}} = \lim_{\xi \rightarrow -\infty} \frac{-1}{1 - e^{a\xi}} = -1,$$

showing that as $\xi \rightarrow -\infty$ this term decays like $-e^{a\xi}$. This yields the claim for $\varkappa = 1$.

Now let $\varkappa \neq 1$, then

$$\eta_\varkappa(e^{a\xi}) = \frac{1}{1 - \varkappa} \ln(e^{\varkappa a \xi} + (1 - e^{a\xi})^\varkappa).$$

Thus (4.38) is evident. Moreover, (4.37) follows from

$$\begin{aligned} \lim_{\xi \rightarrow -\infty} \frac{\eta_\varkappa(e^{a\xi})}{e^{\tilde{\varkappa} a \xi}} &\stackrel{L'H}{=} \frac{\varkappa}{1 - \varkappa} \lim_{\xi \rightarrow -\infty} \frac{\frac{e^{(\varkappa-1)a\xi} - (1 - e^{a\xi})^{\varkappa-1}}{e^{\varkappa a \xi} + (1 - e^{a\xi})^\varkappa} a e^{a\xi}}{a \tilde{\varkappa} e^{\tilde{\varkappa} a \xi}} = \frac{\varkappa}{(1 - \varkappa) \tilde{\varkappa}} \lim_{\xi \rightarrow -\infty} \frac{\frac{e^{\varkappa a \xi} - e^{a\xi}}{e^{\varkappa a \xi} + 1}}{e^{\tilde{\varkappa} a \xi}} \\ &= \frac{\varkappa}{|1 - \varkappa| \tilde{\varkappa}}. \end{aligned}$$

□

4.6. Proof of the Main Result

This section corresponds to [13, Section 8] (with some modifications).

We can now prove our main result.

Proof of Theorem 1.0.1. Having estimated all the error terms in trace norm and knowing that the limiting operator is trace class (see the proof of Theorem 4.4.4), we conclude that the operator

$$\eta_{\varkappa}(\chi_{\mathcal{K}} (\Pi_{\text{BH}}^{(\varepsilon)})_{kn} \chi_{\mathcal{K}}) - \chi_{\mathcal{K}} \eta_{\varkappa}((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}) \chi_{\mathcal{K}}$$

is trace class. Moreover, we saw that all the error terms vanish after dividing by $\ln(1/\varepsilon)$ and taking the limits $u_0 \rightarrow -\infty$ and $\varepsilon \searrow 0$ (in this order). We thus obtain by Corollary 4.4.7,

$$\begin{aligned} & \lim_{\varepsilon \searrow 0} \lim_{u_0 \rightarrow -\infty} \frac{1}{\ln(1/\varepsilon)} \operatorname{tr} \left(\eta_{\varkappa}(\chi_{\mathcal{K}} (\Pi_{\text{BH}}^{(\varepsilon)})_{kn} \chi_{\mathcal{K}}) - \chi_{\mathcal{K}} \eta_{\varkappa}((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}) \chi_{\mathcal{K}} \right) \\ &= \lim_{\varepsilon \searrow 0} \lim_{u_0 \rightarrow -\infty} \frac{1}{\ln(1/\varepsilon)} \operatorname{tr} D_{1/\varepsilon}(\eta_{\varkappa}, \mathcal{K}, \mathfrak{A}^{(0)}) = \frac{1}{\pi^2} U(1; \eta_{\varkappa}) = \frac{1}{\pi^2} \int_0^1 \frac{\eta_{\varkappa}(t)}{t(1-t)} dt. \end{aligned}$$

Moreover since by [29, Appendix],

$$\int_0^1 \frac{\eta_{\varkappa}(t)}{t(1-t)} dt = \frac{\pi^2}{6} \frac{\varkappa + 1}{\varkappa},$$

expressing ε in dimensionless way yields the claim. □

5. The Fermionic Entanglement Entropy of Bounded Regions in Minkowski Space

We begin by noting that in this section, all symbols are independent of \mathbf{x} and \mathbf{y} .

Since for any such measurable and bounded symbol, the integral representation automatically extends to all Schwartz functions (due to Lemma 3.0.2), we will leave out this distinction in this chapter.

Moreover, note that for any \mathbf{x} - and \mathbf{y} -independent symbol $\mathcal{A} \in L^1(\mathbb{R}^d)$, the \mathbf{y} - and ξ -integrals in the definition of $\text{Op}_\alpha(\mathcal{A})$ are interchangeable for any Schwartz function due to Remark 3.0.7.

5.1. The Dirac Equation in Minkowski Spacetime

This section corresponds to [15, Section 2.1] with some parts from [15, Section 1] (both with some modifications).

Minkowski spacetime $(\mathcal{M}, \langle \cdot, \cdot \rangle)$ is described by a real four-dimensional vector space endowed with an inner product $\langle \cdot, \cdot \rangle$ of signature $(+ - - -)$. For \mathcal{M} one may always choose a basis $(e_i)_{i=0, \dots, 3}$ satisfying $\langle e_0, e_0 \rangle = 1$ and $\langle e_i, e_i \rangle = -1$ for $i = 1, 2, 3$. Such a basis is called pseudo-orthonormal basis or *reference frame*, since the corresponding coordinate system (x^i) describes time and space as observed by an observer in a system of inertia. We also refer to $t := x^0$ as time and denote spatial coordinates by $\mathbf{x} = (x^1, x^2, x^3)$. Representing two vectors $x, y \in \mathcal{M}$ in such a basis as $x = \sum_{i=0}^3 x^i e_i$ and $y = \sum_{i=0}^3 y^i e_i$, the inner product takes the form

$$\langle x, y \rangle = \sum_{j,k=0}^3 g_{jk} x^j y^k,$$

where g_{ij} , the *Minkowski metric*, is the diagonal matrix $g = \text{diag}(1, -1, -1, -1)$.

The Dirac equation for a wave function $\psi \in \mathbb{C}^\infty(\mathcal{M}, \mathbb{C}^4)$ of mass $m \geq 0$ in the Minkowski vacuum (i.e. without external potential) reads

$$(i\rlap{/}\partial - m) \psi(x) = 0, \tag{5.1}$$

where we use the slash notation with the Feynman dagger $\rlap{/}\partial := \sum_{j=0}^3 \gamma^j \partial_j$ (for more details on the Dirac equation see [46] or [12, Sections 1.2-1.4]). In this chapter we work with the Dirac matrices in the Dirac representation

$$\gamma^0 = \begin{pmatrix} \mathbf{1}_{\mathbb{C}^2} & 0 \\ 0 & -\mathbf{1}_{\mathbb{C}^2} \end{pmatrix}, \quad \vec{\gamma} = \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix},$$

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and $\vec{\sigma}$ are the three Pauli matrices

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The wave functions at a spacetime point x take values in the *spinor space* S_x , a four-dimensional complex vector space endowed with an indefinite inner product of signature $(2, 2)$, which we call *spin inner product* and denote by

$$\langle \psi | \phi \rangle_x = \sum_{\alpha=1}^4 s_\alpha \psi^\alpha(x)^\dagger \phi^\alpha(x), \quad s_1 = s_2 = 1, \quad s_3 = s_4 = -1,$$

where ψ^\dagger is the complex conjugate wave function (in the physics literature, this inner product is often written as $\bar{\psi}\phi$ with the so-called adjoint spinor $\bar{\psi} = \psi^\dagger \gamma^0$).

Since the Dirac equation is linear and hyperbolic (meaning that it can be rewritten as a symmetric hyperbolic system; for details see for example [12, Chapter 13]), its Cauchy problem for smooth initial data is well-posed, giving rise to global smooth solutions. Moreover, due to finite propagation speed, starting with compactly supported initial data, we obtain solutions which are spatially compact (meaning that their restriction to any Cauchy surface has compact support). Then, the Hilbert space \mathcal{H} is defined as explained in Section 2.1.1 (see (2.2)) by completion of the space of smooth solutions with spatially compact support with respect to the scalar product $(\cdot | \cdot)$ as defined in (2.1). In Minkowski spacetime we choose the Cauchy surface \mathcal{N} in the definition of $(\cdot | \cdot)$ as a surface with fixed time t , such that

$$(\psi | \phi) = \int_{\mathbb{R}^3} \langle \psi | \gamma^0 \phi \rangle_{|_{(t, \mathbf{x})}} d^3 \mathbf{x}. \quad (5.2)$$

In this setting, it is most convenient to write the Dirac equation in an equivalent way which resembles the Schrödinger equation. To this end, we multiply the Dirac equation (5.1) by γ^0 and isolate the t -derivative on one side of the equation,

$$i\partial_t \psi = H\psi \quad \text{where} \quad H := -\gamma^0 (i\vec{\gamma}\vec{\nabla} - m) \quad (5.3)$$

(note that $\sum_{j=0}^3 \gamma^j \partial_j = \gamma^0 \partial_0 + \vec{\gamma}\vec{\nabla}$). The operator H is referred to as the *Dirac Hamiltonian*, and (5.3) is the Dirac equation in the *Hamiltonian form*. By direct computation one verifies that the Hamiltonian is a symmetric operator on the Hilbert space \mathcal{H} . Working at fixed time $t = 0$, in view of (5.2), the Hilbert space \mathcal{H} can be identified with the square-integrable spinors,

$$\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4).$$

In what follows, we shall always work with this identification.

Applying the unitary extension of the Fourier transform \mathcal{F} , the Hamiltonian H may be rewritten as

$$H = \mathcal{F}^{-1} \left(\sum_{\beta=1}^3 k_\beta \gamma^\beta + m \right) \gamma^0 \mathcal{F}.$$

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Using that the Hermitian 4×4 -matrix $(\sum_{\beta=1}^3 k_\beta \gamma^\beta + m) \gamma^0$ is trace-free and that its square can be computed with the help of the anti-commutation relations to be $\mathbf{k}^2 + m^2$ times the identity matrix, we conclude that its eigenvalues are $\pm\sqrt{\mathbf{k}^2 + m^2}$, both with multiplicity two. Hence, diagonalizing this matrix with a suitable unitary matrix S gives

$$\left(\sum_{\beta=1}^3 k_\beta \gamma^\beta + m \right) \gamma^0 = S^{-1} J S \quad \text{with} \quad J := \sqrt{\mathbf{k}^2 + m^2} \operatorname{diag}(-1, -1, 1, 1).$$

Therefore, the projection onto the negative spectral subspace of H is given by

$$\Pi_{\text{MI}} := (S \mathcal{F})^{-1} \frac{1}{2} \left(\mathbb{1} - \frac{1}{\sqrt{\mathbf{k}^2 + m^2}} J \right) S \mathcal{F}. \quad (5.4)$$

Inserting the regularizing factor $e^{-\varepsilon\sqrt{\mathbf{k}^2 + m^2}}$, where $\varepsilon > 0$ is the regularization length we obtain the *regularized projection operator*

$$\begin{aligned} \Pi_{\text{MI}}^{(\varepsilon)} &:= (S \mathcal{F})^{-1} \frac{1}{2} e^{-\varepsilon\sqrt{\mathbf{k}^2 + m^2}} \left(\mathbb{1} - \frac{1}{\sqrt{\mathbf{k}^2 + m^2}} J \right) S \mathcal{F} \\ &= \mathcal{F}^{-1} \frac{1}{2} e^{-\varepsilon\sqrt{\mathbf{k}^2 + m^2}} \left(\mathbb{1} - \frac{(\sum_{\beta=1}^3 k_\beta \gamma^\beta + m) \gamma^0}{\sqrt{\mathbf{k}^2 + m^2}} \right) \mathcal{F}. \end{aligned} \quad (5.5)$$

Changing the variable $\mathbf{k} = \boldsymbol{\xi} \varepsilon^{-1}$ we can rewrite $\Pi_{\text{MI}}^{(\varepsilon)}$ as

$$\Pi_{\text{MI}}^{(\varepsilon)} = \text{Op}_{1/\varepsilon}(\mathcal{A}_{\text{MI}}^{(\varepsilon)}), \quad \text{with} \quad (5.6)$$

$$\mathcal{A}_{\text{MI}}^{(\varepsilon)}(\boldsymbol{\xi}) := \frac{1}{2} \left(\mathbb{1} + \frac{\sum_{\beta=1}^3 \xi_\beta \gamma^\beta - \varepsilon m}{\sqrt{\boldsymbol{\xi}^2 + \varepsilon^2 m^2}} \gamma^0 \right) e^{-\sqrt{\boldsymbol{\xi}^2 + (\varepsilon m)^2}}, \quad (5.7)$$

Rescaling in position space, i.e. applying Lemma 3.0.5 (i) this yields

$$S_{\varkappa}(\Pi_{\text{MI}}^{(\varepsilon)}, L\Lambda) = \text{tr} D_\alpha(\mathcal{A}_{\text{MI}}^{(\varepsilon)}, \Lambda; \eta_\varkappa), \quad \text{where } \alpha = L\varepsilon^{-1}.$$

Remark 5.1.1. (Connection with the kernel of the fermionic projector) For simplicity, we here restrict attention to the Hamiltonian formulation and work exclusively with operators acting on the spatial Hilbert space $L^2(\mathbb{R}^3, \mathbb{C}^4)$. Nevertheless, the operator $\Pi_{\text{MI}}^{(\varepsilon)}$ is closely related to kernels in spacetime, as we now explain. The subspace of negative-energy solutions of Dirac equation in Minkowski spacetime can be described by the *kernel of the fermionic projector* $P^{(\varepsilon)}(x, y)$ defined by

$$P^{(\varepsilon)}(x, y) = \int \frac{1}{(2\pi)^4} \left(\sum_{j=0}^3 k_j \gamma^j + m \right) \delta(\langle k, k \rangle - m^2) \Theta(-k^0) \exp(\varepsilon k^0) e^{-i\langle k, x-y \rangle} d^4 k,$$

where the parameter $\varepsilon > 0$ again describes the regularization (and $\langle \cdot, \cdot \rangle$ is the Minkowski inner product). This kernel plays a central role in the theory of causal fermion systems

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(for more details see [10, Section 2.4.1] or [12, Chapters 15 and 16]). If we choose both arguments on the Cauchy surface $\{t = 0\}$, i.e.

$$x = (0, \mathbf{x}), \quad y = (0, \mathbf{y}) \quad \text{with } \mathbf{x}, \mathbf{y} \in \mathbb{R}^3$$

and carry out the integral over k^0 , we obtain

$$P^{(\varepsilon)}((0, \mathbf{x}), (0, \mathbf{y})) = \frac{1}{(2\pi)^4} \int \frac{1}{2|\omega|} (\not{k} + m) \exp(\varepsilon\omega) \Big|_{\omega = -\sqrt{\mathbf{k}^2 + m^2}} e^{i\mathbf{k}(\mathbf{x}-\mathbf{y})} d^3\mathbf{k}.$$

Comparing with (5.5), one sees that

$$\Pi^{(\varepsilon)}(\mathbf{x}, \mathbf{y}) = -2\pi P^{(\varepsilon)}((0, \mathbf{x}), (0, \mathbf{y})) \gamma^0.$$

Hence the integral kernel of the spatial operator $\Pi_{\text{MI}}^{(\varepsilon)}$ is obtained from the regularized kernel of the fermionic projector simply by multiplying with a prefactor and with the matrix γ^0 from the right. This matrix γ^0 will appear frequently in our formulas; it can be understood as describing the transition from the setting in a Lorentzian spacetime to the purely spatial formulation on a given Cauchy surface. \diamond

5.2. Widom's Formula and its Generalizations

This section is based on [15, Section 3] (with similar phrasing).

In [15] a formula for the asymptotic coefficient was established starting from a result by Widom. In order to state these results, we need to describe first the asymptotic coefficient. For a vector $\mathbf{e} \in \mathbb{S}^{d-1}$, we represent $\boldsymbol{\xi} \in \mathbb{R}^d$ as

$$\boldsymbol{\xi} = \hat{\boldsymbol{\xi}} + t\mathbf{e}, \quad \text{where } t \in \mathbb{R} \text{ and } \hat{\boldsymbol{\xi}} \in \mathbf{T}_{\mathbf{e}} := \{\boldsymbol{\xi} \mid \boldsymbol{\xi} \cdot \mathbf{e} = 0\}.$$

Instead of $\mathcal{A}(\boldsymbol{\xi})$ we sometimes write

$$\mathcal{A}(\hat{\boldsymbol{\xi}}; t) := \mathcal{A}(\hat{\boldsymbol{\xi}} + t\mathbf{e}).$$

For a function $f : \mathbb{R} \rightarrow \mathbb{C}$ denote

$$\mathcal{M}(\hat{\boldsymbol{\xi}}; \mathbf{e}; \mathcal{A}; f) := \text{tr} [\chi_+ f(W_1(\mathcal{A}(\hat{\boldsymbol{\xi}}; \cdot); \mathbb{R}_+)) \chi_+ - W_1(f(\mathcal{A}(\hat{\boldsymbol{\xi}}; \cdot)); \mathbb{R}_+)], \quad \hat{\boldsymbol{\xi}} \in \mathbf{T}_{\mathbf{e}},$$

and introduce

$$\mathfrak{M}(\mathbf{e}; \mathcal{A}; f) := \frac{1}{(2\pi)^{d-1}} \int_{\mathbf{T}_{\mathbf{e}}} \mathcal{M}(\hat{\boldsymbol{\xi}}; \mathbf{e}; \mathcal{A}; f) d\hat{\boldsymbol{\xi}}. \quad (5.8)$$

Finally, denoting the outer unit normal to $\partial\Lambda$ at $\mathbf{x} \in \partial\Lambda$ by $\mathbf{n}_{\mathbf{x}}$, we can define the main asymptotic coefficient:

$$\mathbf{B}(\mathcal{A}; f) := \int_{\partial\Lambda} \mathfrak{M}(\mathbf{n}_{\mathbf{x}}; \mathcal{A}; f) dS_{\mathbf{x}}. \quad (5.9)$$

In what follows we will need the following condition.

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Condition 5.2.1. Let $\mathcal{A} \in C^\infty(\mathbb{R}^d; \mathbb{C}^{n \times n})$, $d \geq 2$, be a matrix-valued symbol (not necessarily Hermitian) such that

$$|\nabla_{\boldsymbol{\xi}}^n \mathcal{A}(\boldsymbol{\xi})| \lesssim \langle \boldsymbol{\xi} \rangle^{-\mu}, \quad n = 0, 1, \dots, \quad \mu > d.$$

Our analysis stems from the following result for smooth symbols \mathcal{A} due to H. Widom [47]. The following is Widom's result stated in the form adapted for our needs.

Proposition 5.2.2. Let $d \geq 2$, and let $\Lambda \subset \mathbb{R}^d$ be a bounded C^1 -region. Suppose that $\mathcal{A} \in C^\infty(\mathbb{R}^d; \mathbb{C}^{n \times n})$ is a matrix-valued symbol satisfying Condition 5.2.1. Let f be a polynomial with $f(0) = 0$. Then

$$\operatorname{tr} f(W_\alpha(\mathcal{A}; \Lambda)) = \left(\frac{\alpha}{2\pi}\right)^d \operatorname{vol}_d(\Lambda) \int_{\mathbb{R}^d} \operatorname{tr} f(\mathcal{A}(\boldsymbol{\xi})) d\boldsymbol{\xi} + \alpha^{d-1} \mathbf{B}(\mathcal{A}; f) + o(\alpha^{d-1}). \quad (5.10)$$

Remark 5.2.3. (i) If the symbol \mathcal{A} is independent of \mathbf{x} and \mathbf{y} and bounded in $\boldsymbol{\xi}$ (as for example in Proposition 5.2.2), we may rewrite $D_\alpha(\mathcal{A}, \Lambda; f)$ due to Lemma 3.0.1 as

$$D_\alpha(\mathcal{A}, \Lambda; f) = \chi_\Lambda f(W_\alpha(\mathcal{A}, \Lambda)) \chi_\Lambda - W_\alpha(f \circ \mathcal{A}, \Lambda). \quad (5.11)$$

(ii) Under the conditions of Proposition 5.2.2 both operators in (5.11) are trace class, and the first term on the right-hand side of (5.10) is exactly $\operatorname{tr} W_\alpha(f \circ \mathcal{A}, \Lambda)$. In this case we also have the equality $\chi_\Lambda f(W_\alpha(\mathcal{A}, \Lambda)) \chi_\Lambda = f(W_\alpha(\mathcal{A}, \Lambda))$, and therefore the formula (5.10) can be rewritten as

$$\lim_{\alpha \rightarrow \infty} \alpha^{1-d} \operatorname{tr} D_\alpha(\mathcal{A}, \Lambda; f) = \mathbf{B}(\mathcal{A}; f). \quad (5.12)$$

On the other hand, if f is a polynomial such that $f(0) \neq 0$, then (5.10) does not make sense, but (5.12) still holds.

(iii) One should mention that in contrast with the matrix case, for scalar symbols $\mathcal{A} = a$ the coefficient $\mathbf{B}(a; f)$ can be found explicitly, see [48] and [50].

In [15] the above result is extended to non-smooth symbols \mathcal{A} and non-smooth functions f . Remembering the relation $\Pi_{\text{MI}}^{(\varepsilon)} = \operatorname{Op}_{1/\varepsilon}(\mathcal{A}_{\text{MI}}^{(\varepsilon)})$ (see (5.6)), the idea was to study symbols that model the symbol $\mathcal{A}_{\text{MI}}^{(\varepsilon)}$ (as defined in (5.7)) and its limit as $\varepsilon \searrow 0$. More precisely, this is mimicked by symbols satisfying the following condition.

Condition 5.2.4. Consider symbols \mathcal{A} that are C^∞ outside of a fixed finite set $\Xi = \{\boldsymbol{\xi}^{(1)}, \boldsymbol{\xi}^{(2)}, \dots, \boldsymbol{\xi}^{(N)}\} \subset \mathbb{R}^d$, and satisfy the bound

$$|\nabla_{\boldsymbol{\xi}}^n \mathcal{A}(\boldsymbol{\xi})| \lesssim \langle \boldsymbol{\xi} \rangle^{-\mu} d(\boldsymbol{\xi})^{-n}, \quad d(\boldsymbol{\xi}) := \min \{ \operatorname{dist}(\boldsymbol{\xi}, \Xi), 1 \}, \quad n = 0, 1, \dots,$$

where $\langle \boldsymbol{\xi} \rangle = \sqrt{1 + |\boldsymbol{\xi}|^2}$.

Moreover, we introduce families of symbols that converge in the following sense.

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Condition 5.2.5. Let $\Xi \subset \mathbb{R}^3$ be a finite set. We assume that the family of Hermitian symbols $\mathcal{A}^{(\varepsilon)} \in C^\infty(\mathbb{R}^d \setminus \Xi; \mathbb{C}^{n \times n})$, $\varepsilon \in [0, 1]$, satisfies the bounds

$$|\nabla_{\xi}^n \mathcal{A}^{(\varepsilon)}(\xi)| \lesssim \langle \xi \rangle^{-\mu} d(\xi)^{-n}, \quad k = 0, 1, \dots,$$

for some $\mu > d$, uniformly in ε . Away from Ξ the symbols $\mathcal{A}^{(\varepsilon)}$ converge to $\mathcal{A} := \mathcal{A}^{(0)}$ uniformly, i.e. for each $h > 0$ we have

$$\sup_{\xi: d(\xi) > h} |\mathcal{A}^{(\varepsilon)}(\xi) - \mathcal{A}(\xi)| \rightarrow 0, \quad \text{as } \varepsilon \searrow 0.$$

Using these conditions we can now state the previously mentioned generalizations of Proposition 5.2.2 from [15]. The first of them deals with fixed non-smooth symbols \mathcal{A} .

Theorem 5.2.6. [15, Theorem 3.4] (adapted to our notation)

Let $d \geq 2$, and let $\Lambda \subset \mathbb{R}^d$ be a bounded C^1 -region. Assume that the function f satisfies Condition 2.2.5 for some $\gamma \in (0, 1]$. Suppose that a Hermitian matrix-valued symbol $\mathcal{A} \in C^\infty(\mathbb{R}^d \setminus \Xi; \mathbb{C}^{n \times n})$ satisfies Condition 5.2.4 for a finite set $\Xi \subset \mathbb{R}^d$ and $\mu > 0$ with $\mu\gamma > d$. Then the formula

$$\lim_{\alpha \rightarrow \infty} \alpha^{1-d} \operatorname{tr} D_\alpha(\mathcal{A}, \Lambda; f) = \mathbf{B}(\mathcal{A}; f) \quad (5.13)$$

holds.

The next theorem considers families of convergent symbols.

Theorem 5.2.7. [15, Theorem 3.5] (adapted to our notation)

Let $d \geq 2$, and let the region $\Lambda \subset \mathbb{R}^d$ and the function f be as in Theorem 5.2.6. Suppose that the family of Hermitian matrix-valued symbols $\mathcal{A}^{(\varepsilon)}$ satisfies Condition 5.2.5 for some $\mu > 0$ with $\mu\gamma > d$. Then, as $\alpha \rightarrow \infty$ and $\varepsilon \searrow 0$, we have

$$\lim \alpha^{1-d} \operatorname{tr} D_\alpha(\mathcal{A}^{(\varepsilon)}, \Lambda; f) = \mathbf{B}(\mathcal{A}; f).$$

5.3. An Abstract Area Law

This section is based on [15, Sections 3 and 7.3] with a result from [15, Section 5.2] (we use similar or sometimes the same phrasing).

As the next Proposition shows, if the symbol \mathcal{A} is “radially symmetric”, then the integral (5.8) is independent of the unit vector \mathbf{e} , which simplifies the expression for the coefficient $\mathbf{B}(\mathcal{A}; f)$ resulting in an abstract area law.

Proposition 5.3.1. [15, Proposition 3.6] (adapted to our notations)

Let $d \geq 2$. Suppose that f satisfies Condition 2.2.5 with some $\gamma \in (0, 1]$, and that $\partial\Lambda$ is a union of finitely many bounded piece-wise C^1 -surfaces. Suppose that a Hermitian matrix-valued symbol $\mathcal{A} \in C^\infty(\mathbb{R}^d \setminus \Xi; \mathbb{C}^{n \times n})$ satisfies Condition 5.2.4 with some $\mu > 0$ such that $\mu\gamma > d$. Suppose also that for each $\mathbf{R} \in \operatorname{SO}(d)$ there exists a matrix $\mathbf{Q} = \mathbf{Q}_{\mathbf{R}} \in \operatorname{SU}(n)$ such that

$$\mathcal{A}(\xi) = \mathbf{Q} \mathcal{A}(\mathbf{R}\xi) \mathbf{Q}^* \quad \text{for a.e. } \xi \in \mathbb{R}^d. \quad (5.14)$$

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Then $\Xi = \{0\}$, and the integral (5.8) does not depend on the vector $\mathbf{e} \in \mathbb{S}^{d-1}$ and

$$\mathbb{B}(\mathcal{A}; f) = \mathfrak{M}(\mathcal{A}; f) \text{vol}_{d-1}(\partial\Lambda), \quad (5.15)$$

where we have denoted $\mathfrak{M}(\mathcal{A}; f) = \mathfrak{M}(\mathbf{e}; \mathcal{A}; f)$ for an arbitrary \mathbf{e} .

The identity $\Xi = \{0\}$ is an immediate consequence of the symmetry (5.14). Indeed if Ξ contained a singular point $\xi_0 \neq 0$, then by (5.14) the symbol \mathcal{A} would have a singularity on the sphere $|\xi| = |\xi_0|$, which is not a finite set.

Note that in Proposition 5.3.1, the region Λ corresponding to the boundary $\partial\Lambda$ does not need to be bounded. In fact, any Λ satisfying the following condition, would be suitable:

Condition 5.3.2. *The set $\Lambda \subset \mathbb{R}^d, d \geq 2$, is a region with piece-wise C^1 -smooth boundary, and either Λ or $\mathbb{R}^d \setminus \Lambda$ is bounded.*

We note that Λ and $\mathbb{R}^d \setminus \bar{\Lambda}$ satisfy Condition 5.3.2 simultaneously. The boundedness of Λ in Theorems 5.2.6 and 5.2.7 is assumed only because both of them are derived from Proposition 5.2.2 where Λ is supposed to be bounded. We remark that many of the intermediate results in [15] hold for the regions satisfying Condition 5.3.2.

For the proof of Proposition 5.3.1 and what follows we will need the following Lemma from [15].

Lemma 5.3.3. *[15, Lemma 5.5] (with slight modifications)*

Let $d \geq 2$. Suppose that f satisfies Condition 2.2.6 with some $\gamma \in (0, 1]$, and Λ satisfies Condition 5.3.2. Moreover, let \mathcal{A} satisfy Condition 5.2.4 with some $\mu > 0$ such that $\mu\gamma > d$. Then for any $\sigma \in (d\mu^{-1}, \gamma)$ we have

$$|\mathcal{M}(\hat{\xi}; \mathbf{e}; \mathcal{A}; f)| \lesssim \|f\|_2 R^{\gamma-\sigma} \langle \hat{\xi} \rangle^{-\mu\sigma+1} \ln(r(\hat{\xi})^{-1} + 2),$$

$$\text{for } \hat{\xi} \in \mathbf{T}_{\mathbf{e}}, \hat{\xi} \notin \hat{\Xi}_{\mathbf{e}},$$

where $\hat{\Xi} = \hat{\Xi}_{\mathbf{e}}$ denotes the projection of the set Ξ onto the hyperplane $\mathbf{T}_{\mathbf{e}}$ and

$$r(\hat{\xi}) = \min \{ \text{dist}(\hat{\xi}, \hat{\Xi}_{\mathbf{e}}), 1 \}.$$

The bound is uniform in \mathcal{A} and $\mathbf{e} \in \mathbb{S}^{d-1}$.

Furthermore,

$$|\mathfrak{M}(\mathbf{e}; \mathcal{A}; f)| \lesssim \|f\|_2 R^{\gamma-\sigma}, \quad (5.16)$$

uniformly in \mathcal{A} and $\mathbf{e} \in \mathbb{S}^{d-1}$, and

$$|\mathbb{B}(\mathcal{A}; f)| \lesssim \|f\|_2 R^{\gamma-\sigma},$$

uniformly in \mathcal{A} . The implicit constants in these bounds do not depend on the set Ξ , but on the number $N = \text{card } \Xi$ only..

We can now prove Proposition 5.3.1.

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Proof of Proposition 5.3.1. First, note that the coefficient $\mathfrak{M}(\mathbf{e}; \mathcal{A}; f)$ is finite by (5.16). Let $\mathbf{e}, \mathbf{b} \in \mathbb{S}^{d-1}$ be two arbitrary unit vectors. Let $\mathbf{R} \in \text{SO}(d)$ be a matrix such that $\mathbf{R}\mathbf{e} = \mathbf{b}$, and let $\mathbf{Q} = \mathbf{Q}_{\mathbf{R}} \in \text{SU}(n)$ be such that (5.14) holds. Thus

$$\mathcal{A}(\hat{\xi}; t) = \mathcal{A}(\hat{\xi} + t\mathbf{e}) = \mathbf{Q}\mathcal{A}(\mathbf{R}\hat{\xi} + t\mathbf{b})\mathbf{Q}^{-1},$$

and hence, by cyclicity of trace, $\mathcal{M}(\hat{\xi}; \mathbf{e}; \mathcal{A}; f) = \mathcal{M}(\mathbf{R}\hat{\xi}; \mathbf{b}; \mathcal{A}; f)$. Integrating in $\hat{\xi}$, we get

$$\begin{aligned} \mathfrak{M}(\mathbf{e}; \mathcal{A}; f) &= \frac{1}{(2\pi)^{d-1}} \int_{\mathbf{T}_{\mathbf{e}}} \mathcal{M}(\mathbf{R}\hat{\xi}; \mathbf{b}; \mathcal{A}; f) d\hat{\xi} \\ &= \frac{1}{(2\pi)^{d-1}} \int_{\mathbf{T}_{\mathbf{b}}} \mathcal{M}(\hat{\xi}; \mathbf{b}; \mathcal{A}; f) d\hat{\xi} = \mathfrak{M}(\mathbf{b}; \mathcal{A}; f). \end{aligned}$$

Thus $\mathfrak{M}(\mathbf{e}; \mathcal{A}; f)$ is indeed \mathbf{e} -independent. Now it is clear that the formula (5.9) rewrites as (5.15), as claimed. \square

5.4. Positivity of the Coefficient $\mathcal{B}(\mathcal{A}; f)$

This section corresponds to [15, Section 8] (with slight modifications).

The goal of this section is to investigate under which conditions on the function f and on the matrix-valued symbol \mathcal{A} the asymptotic coefficient $\mathcal{B}(\mathcal{A}; f)$ defined in (5.9) is strictly positive.

5.4.1. An Abstract Result

Our starting point is the following abstract fact stated in [32, Proposition 3.2] with reference to [28, Theorem A.1] and [4]. Below \mathcal{H} is a complex separable Hilbert space, P an orthogonal projection on \mathcal{H} and A a self-adjoint operator on \mathcal{H} . The operator $\mathcal{D}(A, P; f)$ is defined in (2.9).

Proposition 5.4.1. *Suppose that the spectrum of A is contained in the interval $I \subset \mathbb{R}$, and $f : I \rightarrow \mathbb{R}$ is a concave function. Assume that $\mathcal{D}(A, P; f)$ is trace class and that PAP compact. Then $\text{tr } \mathcal{D}(A, P; f) \geq 0$.*

Using this proposition we can prove the following bound in the spirit of [28, Theorem A.1].

Theorem 5.4.2. *Suppose that the spectrum of A is contained in the interval $I \subset \mathbb{R}$ and that $AP \in \mathbf{S}_2$ and $\mathcal{D}(A, P; f) \in \mathbf{S}_1$. Assume also that $f : I \rightarrow \mathbb{R}$ is a $W_{\text{loc}}^{2,\infty}(I)$ -function such that*

$$\text{ess-sup}_{t \in I} f''(t) = -l_0, \quad \text{with some } l_0 > 0.$$

Then, with the notation $f_0(t) = -\frac{1}{2}t^2$, we have

$$\text{tr } \mathcal{D}(A, P; f) \geq l_0 \text{tr } \mathcal{D}(A, P; f_0) = \frac{l_0}{2} \|(I - P)AP\|_2^2. \quad (5.17)$$

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Proof. We essentially follow the proof of [28, Theorem A.1]. Denote $\mathcal{D}(f) = \mathcal{D}(A, P; f)$ and

$$g(t) = f(t) - l_0 f_0(t),$$

so that $\text{ess-sup}_I g''(t) = 0$. Thus g is concave on I , and by Proposition 5.4.1,

$$\text{tr } \mathcal{D}(f) - l_0 \text{tr } \mathcal{D}(f_0) = \text{tr } \mathcal{D}(g) \geq 0,$$

The first trace on the left-hand side is finite by assumption, and the second one equals

$$2 \text{tr } \mathcal{D}(f_0) = \text{tr} (PA^2P - PAPAP) = \text{tr} (PA(I - P)AP) = \|(I - P)AP\|_2^2,$$

and hence it is also finite. This leads to the required bound (5.17). \square

5.4.2. Application to Pseudo-Differential Operators

Now we can apply the above results to the operator $D_\alpha(\mathcal{A}; f)$. We do not intend to consider the most general functions f satisfying Condition 2.2.5 with some $\gamma \in (0, 1]$, but assume that f is real-valued, the set \mathbf{T} consists of two points, i.e. $\mathbf{T} = \{t_1, t_2\}$ with $t_1 < t_2$, and that

$$\text{ess-sup}_{t \in (t_1, t_2)} f''(t) = -l_0, \quad \text{where } l_0 > 0.$$

We want to prove the following theorem.

Theorem 5.4.3. *Let $d \geq 2$, and let f be as described above. Let $\Lambda \subset \mathbb{R}^d$ be a bounded region with a C^1 -boundary. Suppose that \mathcal{A} is a non-zero Hermitian matrix-valued symbol that satisfies Condition 5.2.4 with some $\mu > 0$ such that $\mu\gamma > d$. Assume also that for all ξ the spectrum of $\mathcal{A}(\xi)$ belongs to the interval $[t_1, t_2]$. Then $\mathbf{B}(\mathcal{A}; f) > 0$.*

We precede the proof with two lemmata.

Lemma 5.4.4. *Let $\mathcal{A} \in C^2(\mathbb{R}; \mathbb{C}^{n \times n})$, be a Hermitian matrix-valued symbol satisfying*

$$\left| \frac{d^l}{d\xi^l} \mathcal{A}(\xi) \right| \lesssim \langle \xi \rangle^{-\mu}, \quad (5.18)$$

for some $\mu > 1$ and $l = 0, 1, 2$. Then the operator $\chi_- \text{Op}_1(\mathcal{A}) \chi_+$ is Hilbert-Schmidt.

If $\mathcal{A}(\xi)$ is a non-zero operator function, the Hilbert-Schmidt norm $\|\chi_- \text{Op}_1(\mathcal{A}) \chi_+\|_2$ is strictly positive.

Proof. Denote the kernel of the operator $\text{Op}_1(\mathcal{A})$ by

$$\check{A}(x) = \frac{1}{2\pi} \int e^{-ix\xi} \mathcal{A}(\xi) d\xi,$$

meaning that for any Schwartz function ψ and almost any $x \in \mathbb{R}$,

$$(\text{Op}_\alpha(\mathcal{A})\psi)(x) = \int_{-\infty}^{\infty} \check{A}(x - y)\psi(y) dy, \quad (5.19)$$

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(due to Remark 3.0.7). Moreover, because of (5.18),

$$|\check{\mathcal{A}}(x)| \lesssim \langle x \rangle^{-2},$$

so by a similar argument as in the proof of Lemma 3.0.6 (applying Hölder's inequality in (5.19) with ψ replaced by $\Delta\psi_n$), we see that the representation (5.19) can be extended to all $\psi \in L^2(\mathbb{R})$.

Then, the (squared) Hilbert-Schmidt norm

$$\begin{aligned} \|\chi_- \text{Op}_1(\mathcal{A})\chi_+\|_2^2 &= \int_{-\infty}^0 \int_0^\infty |\check{\mathcal{A}}(x-y)|^2 dy dx \\ &= \sum_{i,j} \int_{-\infty}^0 \int_0^\infty |\check{\mathcal{A}}_{i,j}(x-y)|^2 dy dx, \end{aligned}$$

is finite. Assume now that there is an interval $I \subset \mathbb{R}$ such that $\mathcal{A}(\xi) \neq 0$ for all $\xi \in I$. Without loss of generality we may assume that the matrix entry $\mathcal{A}_{i,j}(\xi)$ with some i, j , is not zero for all $\xi \in I$. Since \mathcal{A} is Hermitian, we also have

$$\mathcal{A}_{i,j}(\xi) = \overline{\mathcal{A}_{i,j}(\xi)} \neq 0, \quad \xi \in I.$$

As a consequence, $\check{\mathcal{A}}_{i,j}(-x) = \overline{\check{\mathcal{A}}_{i,j}(x)}$, so that the function

$$F(x) := \frac{1}{2} (|\check{\mathcal{A}}_{k,l}(x)|^2 + |\check{\mathcal{A}}_{l,k}(x)|^2)$$

is even and not identically zero. Therefore there is an interval $J \subset \mathbb{R}_-$ such that $F(x) > 0$ for all $x \in J$. Estimating

$$\begin{aligned} \|\chi_- \text{Op}_1(\mathcal{A})\chi_+\|_2^2 &\geq \int_{-\infty}^0 \int_0^\infty F(x-y) dy dx \\ &\geq \int_J \int_{-\infty}^x F(t) dt dx, \end{aligned}$$

we conclude that the Hilbert Schmidt norm on the left-hand side is strictly positive, as required. \square

Using the above lemma we can now show the positivity of the asymptotic coefficient $\mathbf{B}(\mathcal{A}; f_0)$ for the function $f_0(t) = -t^2/2$.

Lemma 5.4.5. *Let $\mathcal{A} \in C^\infty(\mathbb{R}^d \setminus \Xi; \mathbb{C}^{n \times n})$, $d \geq 2$, be a non-zero Hermitian operator-valued symbol satisfying Condition 5.2.4 with $\mu > d$. Then denoting the function $f_0(t) = -t^2/2$ we have $\mathbf{B}(\mathcal{A}; f_0) > 0$.*

Recall that the coefficient $\mathbf{B}(\mathcal{A}; f_0)$ is finite due to Lemma 5.3.3.

Proof. By definition (5.9) it suffices to show that $\mathfrak{M}(\mathbf{e}; \mathcal{A}; f) > 0$ for each $\mathbf{e} \in \mathbb{S}^{d-1}$. Fix a vector \mathbf{e} and rewrite the integrand in (5.8) using the notation $A = \text{Op}_1(\mathcal{A}(\hat{\xi}; \cdot))$, $P = \chi_+$. As in the proof of Theorem 5.4.2, we obtain (also making use of Lemma 3.0.1)

$$2\mathcal{M}(\hat{\xi}; \mathbf{e}; \mathcal{A}; f_0) = \text{tr}(PA^2P - PAPAP) = \text{tr}(PA(I-P)AP) = \|(I-P)AP\|_2^2 \geq 0.$$

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Since \mathcal{A} is a non-zero symbol, there is a ball $\hat{B} \subset \mathbf{T}_e \setminus \hat{\Xi}$ such that for all $\hat{\xi} \in \hat{B}$ the symbol $\mathcal{A}(\hat{\xi}; \cdot)$ is in $C^\infty(\mathbb{R}; \mathbb{C}^{n \times n})$, non-zero and satisfies

$$\left| \frac{d^k}{d\xi^k} \mathcal{A}(\hat{\xi}; \xi) \right| \lesssim \langle \xi \rangle^{-\mu}, \quad k = 0, 1, \dots, \quad \xi \in \mathbb{R},$$

with a constant uniform in $\hat{\xi} \in \hat{B}$. Thus by Lemma 5.4.4, $\mathcal{M}(\hat{\xi}; \mathbf{e}; \mathcal{A}; f_0) > 0$ for all $\hat{\xi} \in \hat{B}$. This leads to the positivity of $\mathbf{B}(\mathcal{A}; f_0)$. \square

5.4.3. Proof of the Positivity of the Limiting Coefficient

Proof of Theorem 5.4.3. In order to use Theorem 5.4.2 we check that $\text{Op}_\alpha(\mathcal{A})\chi_\Lambda$ is Hilbert-Schmidt:

$$\| \text{Op}_\alpha(\mathcal{A})\chi_\Lambda \|_2^2 = \frac{1}{(2\pi\alpha)^d} \int |\mathcal{A}(\xi)|^2 d\xi \int_\Lambda d\mathbf{x} < \infty,$$

where we have used that $|\mathcal{A}(\xi)| \lesssim \langle \xi \rangle^{-\mu}$ with $\mu \geq \mu\gamma > d$. Now, by Theorem 5.4.2,

$$\text{tr } D_\alpha(\mathcal{A}; f) \geq l_0 \text{tr } D_\alpha(\mathcal{A}; f_0), \quad f_0(t) = -\frac{1}{2}t^2.$$

Using the asymptotics (5.13) established in Theorem 5.2.6, we obtain

$$\mathbf{B}(\mathcal{A}; f) \geq l_0 \mathbf{B}(\mathcal{A}; f_0).$$

The latter is positive by Lemma 5.4.5. This completes the proof. \square

5.4.4. Corollaries for the Functions η_\varkappa

Let the functions η_\varkappa be as defined in (1.1). As computed in detail in Lemma C.0.1, each function η_\varkappa satisfies Condition 2.2.5 with $\mathbb{T} = \{0, 1\}$, with $\gamma \leq \min\{\varkappa, 1\}$, if $\varkappa \neq 1$, and $\gamma < 1$ if $\varkappa = 1$.

Corollary 5.4.6. *Let \mathcal{A} and Λ be as in Theorem 5.4.3 and such that $0 \leq \mathcal{A}(\xi) \leq \mathbf{1}$. If $\varkappa \in (0, 2)$, then $\mathbf{B}(\mathcal{A}; \eta_\varkappa) > 0$.*

Proof. By Theorem 5.4.3 it suffices to show that for $\varkappa \in (0, 2)$ the derivative

$$\text{ess-sup}_{t \in (0,1)} \eta_\varkappa''(t) < 0.$$

If $\varkappa = 1$, then one easily finds that $\eta_1''(t) = -t^{-1}(1-t)^{-1} \leq -4$. For $\varkappa \neq 1$ we use a slightly modified version of the proof of [32, Lemma 3.1]. One checks directly that

$$\eta_\varkappa''(t)[t^\varkappa + (1-t)^\varkappa]^2 = -\varkappa[t(1-t)]^{\varkappa-2} - \frac{\varkappa}{1-\varkappa}[t^{\varkappa-1} - (1-t)^{\varkappa-1}]^2. \quad (5.20)$$

For $\varkappa < 1$ the right-hand side is clearly negative for $t \in (0, 1)$ and $\text{ess-sup } \eta_\varkappa''(t) < 0$, as required.

It remains to consider the case $\varkappa \in (1, 2)$. We rewrite (5.20) as

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$$\begin{aligned}\eta''_{\varkappa}(t)[t^{\varkappa} + (1-t)^{\varkappa}]^2 &= -\frac{\varkappa}{\varkappa-1}g_{\varkappa-1}(t), \\ g_p(t) &:= p[t(1-t)]^{p-1} - [t^p - (1-t)^p]^2,\end{aligned}$$

for $p := \varkappa - 1 \in (0, 1)$. Since the term $[t^{\varkappa} + (1-t)^{\varkappa}]^2$ is strictly positive and bounded for $t \in [0, 1]$, it suffices to show that $g_p(t) \geq c$ with some positive c . This claim is equivalent to

$$[t(1-t)]^{1-p}[t^{2p} + (1-t)^{2p} + c] \leq 2t(1-t) + p. \quad (5.21)$$

Using the notation

$$M_p := 2^{p-1} \max_{t \in [0,1]} [t^{2p} + (1-t)^{2p}] = \begin{cases} 2^{-p} & \text{if } 0 < p < 1/2 \\ 2^{p-1} & \text{if } 1/2 \leq p < 1 \end{cases},$$

the (elementary example of the) Young inequality

$$ab \leq \frac{a^u}{u} + \frac{b^v}{v}, \quad a, b \geq 0, \quad u, v > 1, \quad \frac{1}{u} + \frac{1}{v} = 1$$

for $a = [2t(1-t)]^{1-p}$, $u = (1-p)^{-1}$ and $b = 1$, $v = p^{-1}$ yields

$$\begin{aligned}[t(1-t)]^{1-p} [t^{2p} + (1-t)^{2p} + c] &\leq (M_p + 2^{p-1}c)[2t(1-t)]^{1-p} \\ &\leq (M_p + 2^{p-1}c)[(1-p)(2t(1-t)) + p].\end{aligned}$$

Since $M_p < 1$ for $p \in (0, 1)$, the number

$$c = (1 - M_p)2^{1-p}$$

is positive. With this choice of c the above inequality becomes

$$[t(1-t)]^{1-p} [t^{2p} + (1-t)^{2p} + c] \leq (1-p)(2t(1-t)) + p \leq 2t(1-t) + p,$$

so (5.21) holds. This completes the proof of the inequality $\text{ess-sup}_{t \in (0,1)} \eta''_{\varkappa}(t) < 0$ and hence entails that $\mathbf{B}(\mathcal{A}; \eta_{\varkappa}) > 0$. \square

5.5. Proof of the Main Theorem

The main part of this section corresponds to [15, Section 9] with some parts from [15, Section 1] (with slight modifications).

We are now in a position to complete the proof of Theorem 1.0.2. In order to use Theorems 5.2.6 and 5.2.7 we begin with the relation derived already in Section 5.1.

$$S_{\varkappa}(\Pi_{\text{MI}}^{(\varepsilon)}, L\Lambda) = \text{tr } D_{\alpha}(\mathcal{A}_{\text{MI}}^{(\varepsilon)}, \Lambda; \eta_{\varkappa}), \quad \alpha = L\varepsilon^{-1},$$

where the symbol $\mathcal{A}^{(\varepsilon)}$ is given by

$$\mathcal{A}_{\text{MI}}^{(\varepsilon)}(\xi) = \frac{1}{2} \left(\mathbf{1} + \frac{\sum_{\beta=1}^3 \xi_{\beta} \gamma^{\beta} - \varepsilon m}{\sqrt{\xi^2 + \varepsilon^2 m^2}} \gamma^0 \right) e^{-\sqrt{\xi^2 + (\varepsilon m)^2}}.$$

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The symbol $\mathcal{A}_{\text{MI}}^{(\varepsilon)}$ is Hermitian 4×4 -matrix-valued and it satisfies Condition 5.2.5 with the limiting symbol

$$\mathcal{A}_{\text{MI}}(\boldsymbol{\xi}) = \frac{1}{2} \left(\mathbf{1} + \sum_{\beta=1}^3 \frac{\xi_\beta}{|\boldsymbol{\xi}|} \gamma^\beta \gamma^0 \right) e^{-|\boldsymbol{\xi}|}, \quad (5.22)$$

with the finite set $\Xi = \{\mathbf{0}\}$ and for arbitrary $\mu > 0$. Note that in the case $m = 0$, the symbol $\mathcal{A}_{\text{MI}}^{(\varepsilon)}$ coincides with the limiting symbol (5.22) for all $\varepsilon \geq 0$. Moreover, as we have already observed earlier, each function η_\varkappa satisfies Condition 2.2.5 with $\mathbb{T} = \{0, 1\}$, with $\gamma \leq \min\{\varkappa, 1\}$, if $\varkappa \neq 1$, and $\gamma < 1$ if $\varkappa = 1$ (see also Lemma C.0.1). Thus, according to Theorem 5.2.6, as $L \rightarrow \infty$ and $\varepsilon > 0$ is fixed, we have

$$\lim (L\varepsilon^{-1})^{-2} S_\varkappa(\Pi_{\text{MI}}^{(\varepsilon)}, L\Lambda) = \lim \alpha^{-2} \text{tr} D_\alpha(\mathcal{A}_{\text{MI}}^{(\varepsilon)}, \Lambda; \eta_\varkappa) = \mathbf{B}(\mathcal{A}_{\text{MI}}^{(\varepsilon)}; \eta_\varkappa),$$

for any bounded \mathbb{C}^1 -region $\Lambda \subset \mathbb{R}^3$. Similarly, if $\varepsilon \searrow 0$ and $\alpha = L\varepsilon^{-1} \rightarrow \infty$, then Theorem 5.2.7 leads to the formula

$$\lim L^{-2} \varepsilon^2 S_\varkappa(\Pi_{\text{MI}}^{(\varepsilon)}, L\Lambda) = \mathbf{B}(\mathcal{A}_{\text{MI}}; \eta_\varkappa),$$

for any bounded \mathbb{C}^1 -region $\Lambda \subset \mathbb{R}^3$. To complete the proof of (1.7) and (1.8) we will check that the symbols $\mathcal{A}^{(\varepsilon)}, \mathcal{A}$ satisfy the conditions of Proposition 5.3.1. The following lemma is the first step in this direction.

Lemma 5.5.1. *Let $\mathbf{R} \in \text{SO}(3)$ be arbitrary. Then there exists a matrix $\mathbf{Q} = \mathbf{Q}_{\mathbf{R}} \in \text{SU}(4)$ such that for any $\mathbf{v} \in \mathbb{R}^3$:*

$$\mathbf{Q} \sum_{\beta=1}^3 (\mathbf{R}\mathbf{v})_\beta \gamma^\beta \mathbf{Q}^{-1} = \sum_{\beta=1}^3 v_\beta \gamma^\beta, \quad \text{and} \quad \mathbf{Q} \gamma^0 \mathbf{Q}^{-1} = \gamma^0.$$

Proof. The foundation for this proof can for example be found in [12, Lemma 1.3.1 and its proof].

It suffices to prove this lemma for rotations around the three coordinate axes, since any other rotation may be written as a product of those three rotations.

Without loss of generality assume that \mathbf{R} is a rotation around the z -axis. Then it is given by

$$\mathbf{R} = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

where $\theta \in \mathbb{R}$ is the rotation angle. We claim that

$$\mathbf{Q} := \begin{pmatrix} e^{-i\theta/2} & & & \\ & e^{i\theta/2} & & \\ & & e^{-i\theta/2} & \\ & & & e^{i\theta/2} \end{pmatrix}$$

is the sought matrix. Indeed, note that

$$\mathbf{Q} \gamma^0 \mathbf{Q}^{-1} = \gamma^0, \quad \mathbf{Q} \gamma^3 \mathbf{Q}^{-1} = \gamma^3,$$

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$$\mathbf{Q} \gamma^1 \mathbf{Q}^{-1} = \begin{pmatrix} & & e^{i\theta} \\ & -e^{-i\theta} & \\ -e^{-i\theta} & & \end{pmatrix},$$

$$\mathbf{Q} \gamma^2 \mathbf{Q}^{-1} = \begin{pmatrix} & & -ie^{i\theta} \\ & ie^{-i\theta} & \\ -ie^{-i\theta} & & \end{pmatrix}.$$

Then, by a straightforward computation we see that

$$\begin{aligned} & \mathbf{Q} \sum_{\beta=1}^3 (\mathbf{R}\mathbf{v})_{\beta} \gamma^{\beta} \mathbf{Q}^{-1} \\ &= v_1 \left(\cos \theta \mathbf{Q} \gamma^1 \mathbf{Q}^{-1} + \sin \theta \mathbf{Q} \gamma^2 \mathbf{Q}^{-1} \right) + v_2 \left(-\sin \theta \mathbf{Q} \gamma^1 \mathbf{Q}^{-1} + \cos \theta \mathbf{Q} \gamma^2 \mathbf{Q}^{-1} \right) \\ & \quad + v_3 \gamma^3 = \sum_{\beta=1}^3 v_{\beta} \gamma^{\beta}, \end{aligned}$$

which concludes the proof. \square

Lemma 5.5.1 ensures that the symbols \mathcal{A}_{MI} and $\mathcal{A}_{\text{MI}}^{(\varepsilon)}$ satisfy the conditions of Proposition 5.3.1. Therefore for any bounded C^1 -region Λ with finitely many connected components,

$$\mathbf{B}(\mathcal{A}_{\text{MI}}^{(\varepsilon)}; \eta_{\varkappa}) = \mathfrak{M}_{\varkappa}^{(\varepsilon)} \text{vol}_2(\partial\Lambda), \quad \mathbf{B}(\mathcal{A}_{\text{MI}}; \eta_{\varkappa}) = \mathfrak{M}_{\varkappa} \text{vol}_2(\partial\Lambda),$$

where

$$\mathfrak{M}_{\varkappa}^{(\varepsilon)} := \mathfrak{M}(\mathbf{e}; \mathcal{A}_{\text{MI}}^{(\varepsilon)}; \eta_{\varkappa}), \quad \mathfrak{M}_{\varkappa} := \mathfrak{M}(\mathbf{e}; \mathcal{A}_{\text{MI}}; \eta_{\varkappa}),$$

with an arbitrary unit vector \mathbf{e} . The convergence $\mathfrak{M}_{\varkappa}^{(\varepsilon)} \rightarrow \mathfrak{M}_{\varkappa}$ as $\varepsilon \searrow 0$, follows from the next lemma from [15].

Lemma 5.5.2. [15, Lemma 7.2] *Let f and Λ be as in Theorem 5.2.6, and let the family $\mathcal{A}^{(\varepsilon)}$ satisfy Condition 5.2.5. Then*

$$\mathbf{B}(\mathcal{A}^{(\varepsilon)}; f) \rightarrow \mathbf{B}(\mathcal{A}; f), \quad \text{as } \varepsilon \searrow 0.$$

Finally, since the matrix symbols \mathcal{A}_{MI} and $\mathcal{A}_{\text{MI}}^{(\varepsilon)}$ satisfy the bounds $0 \leq \mathcal{A}_{\text{MI}}(\boldsymbol{\xi}) \leq \mathbf{1}$ and $0 \leq \mathcal{A}_{\text{MI}}^{(\varepsilon)}(\boldsymbol{\xi}) \leq \mathbf{1}$ for all $\boldsymbol{\xi}$, it follows from Corollary 5.4.6 that $\mathbf{B}(\mathcal{A}_{\text{MI}}; \eta_{\varkappa}) > 0$ and $\mathbf{B}(\mathcal{A}_{\text{MI}}^{(\varepsilon)}; \eta_{\varkappa}) > 0$ for $\varkappa \in (0, 2)$. This immediately implies that $\mathfrak{M}_{\varkappa}^{(\varepsilon)} > 0$ and $\mathfrak{M}_{\varkappa} > 0$ for $\varkappa \in (0, 2)$, as claimed. The proof of Theorem 1.0.2 is now complete.

6. Summary and Outlook

We finally summarize this thesis and give some perspectives for future research. The first part of this section is based on [13, Section 9] (with some modifications) moreover some of the remaining section is based on [15, Sections 1 and 3].

In the Schwarzschild case we introduced the Rényi entanglement entropy of a Schwarzschild black hole horizon based on the Dirac propagator as

$$S_{\varkappa}^{\text{BH}} = \frac{1}{2} \sum_{\substack{(k,n) \\ \text{occupied}}} \lim_{\varepsilon \searrow 0} \lim_{u_0 \rightarrow -\infty} \frac{1}{\ln(M/\varepsilon)} \text{tr} \left(\eta_{\varkappa} (\chi_{\mathcal{K}} (\Pi_{\text{BH}}^{(\varepsilon)})_{kn} \chi_{\mathcal{K}}) - \chi_{\mathcal{K}} \eta_{\varkappa} ((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}) \chi_{\mathcal{K}} \right), \quad (6.1)$$

(we left out the ρ -limit here since we have seen, that the ρ -dependence drops out after taking the u_0 - and ε -limits). We have shown that we may treat each angular mode separately. This transition enables us to disregard the angular coordinates, which makes the problem essentially one-dimensional in space. Furthermore, in the limiting case we were able to replace the symbol of the corresponding pseudo-differential operator by $\mathfrak{A}^{(0)}$ in (4.16) provided that $\varkappa > \frac{2}{3}$. Since this symbol is diagonal matrix-valued, this reduces the problem to one spin dimension. Moreover, because $\mathfrak{A}^{(0)}$ is also independent of ε , the trace with the replaced symbol can be computed explicitly. It turns out to be a numerical constant independent of the considered angular mode.

This leads us to the conclusion that the fermionic entanglement entropy of the horizon is proportional to the number of angular modes occupied at the horizon,

$$S_1^{\text{BH}} = \sum_{\substack{(k,n) \\ \text{occupied}}} S_{1,kn}^{\text{BH}} = \frac{1}{6} \#\{(k,n) \mid \text{angular mode } (k,n) \text{ occupied}\},$$

and a similar result holds for the Rényi entropies with $\varkappa > \frac{2}{3}$. This is comparable to the counting of states in string theory [42] and loop quantum gravity [2]. Furthermore, assuming that there is a minimal area of order ε^2 , the number of occupied modes at the horizon were given by M^2/ε^2 , which would lead to

$$S_1^{\text{BH}} = \frac{1}{6} \frac{M^2}{\varepsilon^2}.$$

Bringing the factor $\ln(M/\varepsilon)$ in (6.1) to the other side, this would mean that, up to lower orders in ε^{-1} , we would obtain the enhanced area law

$$\begin{aligned} & \sum_{\substack{(k,n) \\ \text{occupied}}} \lim_{u_0 \rightarrow -\infty} \text{tr} \left(\eta (\chi_{\Lambda} (\Pi_{\text{BH}}^{(\varepsilon)})_{kn} \chi_{\Lambda}) - \chi_{\Lambda} \eta ((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}) \chi_{\Lambda} \right) \\ &= \frac{1}{6} \frac{M^2}{\varepsilon^2} \ln(M/\varepsilon) + o(M^2/\varepsilon^2 \ln(M/\varepsilon)), \quad \text{as } \varepsilon \searrow 0. \end{aligned}$$

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An interesting topic for future research would be to determine the number of occupied angular momentum modes at the horizon in more detail, for example by considering a collapse model.

Moreover, since initially we only had the entanglement entropy (i.e. the case $\varkappa = 1$) in mind, we only established estimates for R^\pm and its first derivative in u . This had the consequence that we were not able to estimate the corresponding error terms for Rényi entropies with $\varkappa \leq \frac{2}{3}$ with the same methods. However, those methods would in principle also apply for $\varkappa \leq \frac{2}{3}$ as well if suitable estimates for higher derivatives of R^\pm were worked out. This is another topic for future research.

In the second part of this thesis we considered the Rényi entanglement entropy operator $S_\varkappa(\Pi_\varepsilon^{\text{MI}}, L\Lambda)$ of bounded spatial regions $L\Lambda$ with C^1 -boundary and finitely many connected components in Minkowski spacetime. We considered two limiting cases. The first where L is kept fixed and the regularization tends to zero, which is the usual definition of entanglement entropy. Furthermore we considered the case where the regularization is fixed and the parameter L describing the size of $L\Lambda$ tends to infinity. This gives under the assumption of a fixed regularization (for example when identifying it with the Planck length) the behavior of the entanglement entropy when the volume gets larger and larger. We started by rewriting $\Pi_{\text{MI}}^{(\varepsilon)}$ as pseudo-differential operator and then applying results from [15] to obtain the limiting coefficient. The symmetry of the Dirac equation then allowed us to factor out the area and finally the strict concavity of the function η_\varkappa for $0 < \varkappa < 2$ together with a result going back to Berezin from [4] lead to the positivity of the Rényi entanglement entropy. This resulted in an area law for the Rényi entanglement entropies in both limiting cases. Namely in the first case where $L\varepsilon^{-1} \rightarrow \infty$ and $\varepsilon \searrow 0$

$$\lim L^{-2}\varepsilon^2 S_\varkappa(\Pi_{\text{MI}}^{(\varepsilon)}, L\Lambda) = \mathfrak{M}_\varkappa \text{vol}_2(\partial\Lambda),$$

where \mathfrak{M}_\varkappa is an explicit constant. And for $L \rightarrow \infty$ and $\varepsilon > 0$ is fixed,

$$\lim L^{-2}\varepsilon^2 S_\varkappa(\Pi_{\text{MI}}^{(\varepsilon)}, L\Lambda) = \mathfrak{M}_\varkappa^{(\varepsilon)} \text{vol}_2(\partial\Lambda).$$

where $\mathfrak{M}_\varkappa^{(\varepsilon)}$ is some explicit constant such that $\mathfrak{M}_\varkappa^{(\varepsilon)} \rightarrow \mathfrak{M}_\varkappa$ as $\varepsilon \rightarrow 0$. Moreover, for $0 < \varkappa < 2$, both coefficients \mathfrak{M}_\varkappa and $\mathfrak{M}_\varkappa^{(\varepsilon)}$ are strictly positive.

Since as mentioned before, many interim results in [15] hold for any region satisfying Condition 5.3.2, an interesting topic for future research would be to investigate if a similar result holds for unbounded regions Λ satisfying Condition 5.3.2.

A. Proof of Lemma 4.1.2

We follow the proof of [11, Lemma 3.1]. As explained there, employing the ansatz

$$X(u) = \begin{pmatrix} e^{-i\omega u} f^+(u) \\ e^{i\omega u} f^-(u) \end{pmatrix}, \quad (\text{A.1})$$

the vector-valued function f must satisfy the ODE

$$\frac{d}{du} f = \frac{\sqrt{\Delta(r)}}{r^2} \begin{pmatrix} 0 & e^{2i\omega u} (imr - \lambda) \\ e^{-2i\omega u} (-imr - \lambda) & 0 \end{pmatrix} f, \quad (\text{A.2})$$

where λ is an eigenvalue of the operator

$$\mathcal{A} := \begin{pmatrix} 0 & \frac{d}{d\vartheta} + \frac{\cot \vartheta}{2} + \frac{k+1/2}{\sin \vartheta} \\ -\frac{d}{d\vartheta} - \frac{\cot \vartheta}{2} + \frac{k+1/2}{\sin \vartheta} & 0 \end{pmatrix}$$

(see [11, Appendix A]) and thus does not depend on ω (in contrast to the Kerr-Newman case as explained in [11, Appendix A]). Estimating (A.2) gives

$$\left| \frac{d}{du} f \right| \leq \left| \frac{\sqrt{r-2M}}{r^{3/2}} \right| (mr + |\lambda|) |f| = \sqrt{\frac{r-2M}{r}} \left(m + \frac{|\lambda|}{r} \right) |f|.$$

Next, we transform $r - 2M$ to the Regge-Wheeler-coordinate,

$$r - 2M = 2M W(e^{u/(2M)-1}/2M),$$

where W is the inverse log function, i.e. the inverse function of $x \mapsto xe^x$. An elementary estimate⁷ shows that $0 \leq W(x) \leq x$ for any $x \geq 0$ and therefore we can estimate

$$\left| \frac{d}{du} f \right| \leq e^{u/2M-1} \left(m + \frac{|\lambda|}{2M} \right) |f|. \quad (\text{A.3})$$

Setting

$$c_1 := \frac{1}{e} \left(m + \frac{|\lambda|}{2M} \right), \quad d := \frac{1}{2M},$$

we can proceed just as in [11, Proof of 3.1]:

Without loss of generality we can assume that $|f|$ is nowhere vanishing⁸ and divide (A.3) by $|f|$ giving

$$\frac{|d/du f|}{|f|} \leq c_1 e^{du}.$$

⁷Since the function $f(x) := xe^x$ is strictly increasing (and differentiable) on $(0, \infty)$, so is $W = f^{-1}$ on $(f(0), f(\infty)) = (0, \infty)$. So from $xe^x \geq x$ for any $x \geq 0$ follows $x = W(xe^x) \geq W(x)$. Moreover, due to the monotony and since $W(0) = 0$, we have $W(x) \geq 0$ for any $x \geq 0$.

⁸If $f(\tilde{u}) = 0$ for one $\tilde{u} \in \mathbb{R}$, then due to (A.2) also $(\frac{df}{du})|_{\tilde{u}} = 0$ and thus by the Picard-Lindelöf theorem, f vanishes identically on \mathbb{R} .

A. Proof of Lemma 4.1.2

This yields for any $u < u_2$,

$$\begin{aligned} |\ln(|f(u_2)|) - \ln(|f(u)|)| &= \left| \int_u^{u_2} \frac{\frac{d}{du} (|f^+(u')|^2 + |f^-(u')|^2)}{|f(u')|^2} du' \right| \leq 4 \int_u^{u_2} c_1 e^{du'} du' \\ &= \frac{4c_1}{d} (e^{du_2} - e^{du}). \end{aligned}$$

From this we conclude that

$$\begin{aligned} \ln(|f(u)|) &\geq \ln(|f(u_2)|) - \frac{4c_1}{d} (e^{du_2} - e^{du}) \geq \ln(|f(u_2)|) - \frac{4c_1}{d} e^{du_2} \\ \ln(|f(u)|) &\leq \ln(|f(u_2)|) + \frac{4c_1}{d} (e^{du_2} - e^{du}) \leq \ln(|f(u_2)|) + \frac{4c_1}{d} e^{du_2}, \end{aligned}$$

which yields

$$|f(u_2)| \exp\left(-\frac{4c_1}{d} e^{du_2}\right) \leq |f(u)| \leq |f(u_2)| \exp\left(\frac{4c_1}{d} e^{du_2}\right). \quad (\text{A.4})$$

Using this inequality in (A.3), we obtain

$$\left| \frac{d}{du} f \right| \leq c_1 |f(u_2)| \exp\left(\frac{4c_1}{d} e^{du_2}\right) e^{du}, \quad (\text{A.5})$$

which shows that $\frac{df}{du}$ is integrable. Moreover due to (A.4), $f(u)$ converges for $u \rightarrow -\infty$ to

$$f_0 := \lim_{u \rightarrow -\infty} f(u) \stackrel{(\text{A.4})}{\neq} 0.$$

Now integrating (A.5) from $-\infty$ to $u < u_2$, we get

$$|f(u) - f_0| \leq \frac{c_1}{d} |f(u_2)| \exp\left(\frac{4c_1}{d} e^{du_2}\right) e^{du}. \quad (\text{A.6})$$

Finally, in order to get rid of the factor $|f(u_2)|$, we make use of (A.4) in the limit $u \rightarrow -\infty$,

$$|f(u_2)| \leq |f_0| \exp\left(\frac{4c_1}{d} e^{du_2}\right). \quad (\text{A.7})$$

Substituting this in (A.6), we end up with the desired result

$$|g(u)| \leq ce^{du},$$

with

$$g(u) := f(u) - f_0, \quad \text{and} \quad c := \frac{c_1}{d} |f_0| \exp\left(\frac{8c_1}{d} e^{du_2}\right).$$

Similarly, removing $|f(u_2)|$ from (A.5) using (A.7) we obtain

$$\left| \frac{d}{du} g \right| \leq dce^{du},$$

which completes the proof. \square

B. Computing the Symbol of $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$

In this section, we give a more detailed computation of the symbol of the operator $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$ for given k and n . Recall that $(\Pi_{\text{BH}}^{(\varepsilon)})_{kn}$ is for any function $\psi \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$ given by,

$$((\Pi_{\text{BH}}^{(\varepsilon)})_{kn}\psi)(u) = \frac{1}{\pi} \int d\omega \int du' e^{-\varepsilon\omega} \sum_{a,b=1}^2 t_{a,b}^\omega X_a(u, \omega) \langle X_b(\cdot, \omega) | \psi \rangle.$$

The main task is therefore to determine

$$\sum_{a,b=1}^2 t_{a,b}^\omega X_a(u, \omega) X_b(u', \omega)^\dagger =: (*). \quad (\text{B.1})$$

To this end first note that the details of the coefficients t_{ab} in (4.2) give

$$(*) = \chi_{(-m,0)}(\omega) X_1(u, \omega) X_1(u', \omega)^\dagger \quad (\text{B.2})$$

$$+ \chi_{(-\infty, -m)}(\omega) \left[\frac{1}{2} X_1(u, \omega) X_1(u', \omega)^\dagger + \frac{1}{2} X_2(u, \omega) X_2(u', \omega)^\dagger \right. \quad (\text{B.3})$$

$$\left. + t_{12}^\omega X_1(u, \omega) X_2(u', \omega)^\dagger + t_{21}^\omega X_2(u, \omega) X_1(u', \omega)^\dagger \right]. \quad (\text{B.4})$$

Moreover, using the asymptotics of the radial solutions given in Lemma 4.1.2 the matrix $X_a(u, \omega) X_b(u', \omega)^\dagger$ can for any $a, b \in \{1, 2\}$ be written as

$$\begin{aligned} & X_a(u, \omega) X_b(u', \omega)^\dagger \\ &= \begin{pmatrix} f_{0,a}^+(\omega) \overline{f_{0,b}^+(\omega)} e^{-i\omega(u-u')} & f_{0,a}^+(\omega) \overline{f_{0,b}^-(\omega)} e^{-i\omega(u+u')} \\ f_{0,a}^-(\omega) \overline{f_{0,b}^+(\omega)} e^{i\omega(u+u')} & f_{0,a}^-(\omega) \overline{f_{0,b}^-(\omega)} e^{i\omega(u-u')} \end{pmatrix} \end{aligned} \quad (\text{B.5})$$

$$+ R_{0,a}(u, \omega) \begin{pmatrix} f_{0,b}^+(\omega) e^{-i\omega u'} \\ f_{0,b}^-(\omega) e^{i\omega u'} \end{pmatrix}^\dagger + \begin{pmatrix} f_{0,a}^+(\omega) e^{-i\omega u} \\ f_{0,a}^-(\omega) e^{i\omega u} \end{pmatrix} R_{0,b}(u', \omega)^\dagger \quad (\text{B.6})$$

$$+ R_{0,a}(u, \omega) R_{0,b}(u', \omega)^\dagger. \quad (\text{B.7})$$

Where by $f_{0,a}^\pm$ and $R_{0,a}$ we denote the functions f_0^\pm and R_0 corresponding to X_a for each $a = 1, 2$. The terms in (B.6)-(B.7) will result in the error matrix $\mathcal{R}_{0,\varepsilon}$ and will be computed in Section 4.5.1. Here we are mainly interested in the terms in (B.5).

Combining our choices of f_0 from Section 4.1.4 with (B.5) and (B.2)-(B.4), we obtain

$$\begin{aligned} (*) &= \chi_{(-m,0)}(\omega) \begin{pmatrix} |f_{0,1}^+(\omega)|^2 e^{-i\omega(u-u')} & f_{0,1}^+(\omega) \overline{f_{0,1}^-(\omega)} e^{-i\omega(u+u')} \\ f_{0,1}^-(\omega) \overline{f_{0,1}^+(\omega)} e^{i\omega(u+u')} & |f_{0,1}^-(\omega)|^2 e^{i\omega(u-u')} \end{pmatrix} \\ &+ \chi_{(-\infty, -m)}(\omega) \begin{pmatrix} \frac{1}{2} e^{-i\omega(u-u')} & t_{12}^\omega e^{-i\omega(u+u')} \\ t_{21}^\omega e^{i\omega(u+u')} & \frac{1}{2} e^{i\omega(u-u')} \end{pmatrix} + \tilde{\mathcal{R}}_0(u, u', \omega), \end{aligned}$$

B. Computing the Symbol of $(\Pi_{BH}^{(\varepsilon)})_{kn}$

where $\tilde{\mathcal{R}}_0(u, u', \omega)$ consists of the terms (B.6)-(B.7) inserted in the sum (B.1).

In order to rewrite $(\Pi_{BH}^{(\varepsilon)})_{kn}$ as a pseudo-differential operator, we need a prefactor of the form $e^{-i\omega(u-u')}$ before the symbol. The matrix components in (*) indeed involve such plane waves. However, the (2, 2)-components oscillate with the wrong sign. In order to circumvent this issue, we can use the freedom of coordinate change $\omega \rightarrow -\omega$ in the $d\omega$ integration of the (2, 2) and (1, 2) components. This yields (4.10).

C. Regularity of the Functions η_\varkappa

We now verify in detail that the functions η_\varkappa satisfy Condition 2.2.5.

Lemma C.0.1. *Consider the functions η_\varkappa in (1.1). Then for any $\varkappa \neq 1$, η_\varkappa satisfies Condition 2.2.5 with $\mathbb{T} = \{0, 1\}$ for any $\gamma \leq \min\{\varkappa, 1\}$. Moreover, $\eta = \eta_1$ satisfies Condition 2.2.5 with $\mathbb{T} = \{0, 1\}$ for any $\gamma < 1$.*

Proof. We start with the case that $\varkappa = 1$. Then, in order to prove that

$$\eta \in \mathcal{C}^2(\mathbb{R} \setminus \{0, 1\}) \cap \mathcal{C}^0(\mathbb{R}),$$

it suffices to show the continuity at $t = 0$ and $t = 1$, which follows from

$$\lim_{t \searrow 0} (-t \ln(t) - (1-t) \ln(1-t)) = -\lim_{t \searrow 0} \frac{\ln(t)}{t^{-1}} \stackrel{L'H}{=} \lim_{t \searrow 0} \frac{t^{-1}}{t^{-2}} = 0,$$

(where “L’H” denotes the use of L’Hôpital’s rule) and

$$\lim_{t \nearrow 1} (-t \ln(t) - (1-t) \ln(1-t)) = -\lim_{t \nearrow 1} \frac{\ln(1-t)}{(1-t)^{-1}} \stackrel{L'H}{=} \lim_{t \nearrow 1} \frac{(1-t)^{-1}}{(1-t)^{-2}} = 0.$$

Moreover, for any $t \in (0, 1)$ we have

$$\begin{aligned} \eta'(t) &= -\ln(t) + \ln(1-t), \\ \eta''(t) &= -\frac{1}{t} - \frac{1}{1-t}. \end{aligned}$$

Thus, for any $\gamma < 1$

$$\begin{aligned} \lim_{t \searrow 0} \eta(t)t^{-\gamma} &= -\lim_{t \searrow 0} \frac{\ln t}{t^{\gamma-1}} - \lim_{t \searrow 0} \frac{\ln(1-t)}{t^\gamma} \stackrel{L'H}{=} -\lim_{t \searrow 0} \frac{t^{-1}}{(\gamma-1)t^{\gamma-2}} + \lim_{t \searrow 0} \frac{(1-t)^{-1}}{\gamma t^{\gamma-1}} \\ &= \lim_{t \searrow 0} \frac{t^{1-\gamma}}{1-\gamma} + \lim_{t \searrow 0} \frac{t^{1-\gamma}}{\gamma(1-t)} = 0, \end{aligned}$$

and obviously

$$\lim_{t \nearrow 0} \eta(t)t^{-\gamma} = 0.$$

Therefore, there exists a neighborhood $U_{0,0}$ of $t_0 = 0$ and a constant $C_{0,0}$ such that for any $t \in U_{0,0}$,

$$|\eta(t)| \leq C_{0,0}|t|^\gamma.$$

Similarly we obtain for $t_1 = 1$,

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$$\begin{aligned} \lim_{t \nearrow 1} \eta(t)(1-t)^{-\gamma} &= -\lim_{t \nearrow 1} \frac{\ln t}{(1-t)^\gamma} - \lim_{t \nearrow 1} \frac{\ln(1-t)}{(1-t)^{\gamma-1}} \\ &\stackrel{L'H}{=} \lim_{t \nearrow 1} \frac{t^{-1}}{\gamma(1-t)^{\gamma-1}} - \lim_{t \nearrow 1} \frac{(1-t)^{-1}}{(\gamma-1)(1-t)^{\gamma-2}} = 0, \\ \lim_{t \searrow 1} \eta(t)(1-t)^{-\gamma} &= 0, \end{aligned}$$

yielding a neighborhood $U_{1,0}$ of $t_1 = 1$ and a constant $C_{1,0}$ such that for any $t \in U_{1,0}$:

$$|\eta(t)| \leq C_{1,0} |t-1|^\gamma.$$

The other estimates follow analogously by computing the limits

$$\begin{aligned} \lim_{t \searrow 0} \eta'(t)t^{1-\gamma} &= -\lim_{t \searrow 0} \frac{\ln(t)}{t^{\gamma-1}} \stackrel{L'H}{=} \lim_{t \searrow 0} \frac{t^{-1}}{(1-\gamma)t^{\gamma-2}} = \lim_{t \searrow 0} \frac{t^{1-\gamma}}{1-\gamma} = 0, \\ \lim_{t \nearrow 1} \eta'(t)(1-t)^{1-\gamma} &= \lim_{t \nearrow 1} \frac{\ln(1-t)}{(1-t)^{\gamma-1}} \stackrel{L'H}{=} \lim_{t \nearrow 1} \frac{(1-t)^{-1}}{(\gamma-1)(1-t)^{\gamma-2}} = \lim_{t \nearrow 1} \frac{(1-t)^{1-\gamma}}{\gamma-1} = 0, \\ \lim_{t \searrow 0} \eta''(t)t^{2-\gamma} &= -\lim_{t \searrow 0} t^{1-\gamma} = 0, \\ \lim_{t \nearrow 1} \eta''(t)(1-t)^{2-\gamma} &= -\lim_{t \nearrow 1} (1-t)^{1-\gamma} = 0, \\ \lim_{t \nearrow 0} \eta'(t)t^{1-\gamma} &= \lim_{t \searrow 1} \eta'(t)(1-t)^{1-\gamma} = \lim_{t \nearrow 0} \eta''(t)t^{2-\gamma} = \lim_{t \searrow 1} \eta''(t)(1-t)^{2-\gamma} = 0. \end{aligned}$$

This concludes the proof for the case that $\varkappa = 1$.

Next, consider $\varkappa \neq 1$. It is evident that

$$\eta_{\varkappa} \in \mathcal{C}^2(\mathbb{R} \setminus \{0, 1\}) \cap \mathcal{C}^0(\mathbb{R}).$$

Moreover, note that for any $\gamma \leq \varkappa$,

$$\begin{aligned} \lim_{t \searrow 0} \frac{\eta_{\varkappa}(t)}{t^\gamma} &= \frac{1}{1-\varkappa} \lim_{t \searrow 0} \frac{\ln(t^\varkappa + 1)}{t^\gamma} \stackrel{L'H}{=} \frac{\varkappa}{1-\varkappa} \lim_{t \searrow 0} \frac{(t^\varkappa + 1)^{-1} t^{\varkappa-1}}{t^{\gamma-1}} \\ &= \frac{\varkappa}{1-\varkappa} \lim_{t \searrow 0} t^{\varkappa-\gamma} < \infty, \\ \lim_{t \nearrow 1} \frac{\eta_{\varkappa}(t)}{(1-t)^\gamma} &= \frac{1}{1-\varkappa} \lim_{t \nearrow 1} \frac{\ln(1 + (1-t)^\varkappa)}{(1-t)^\gamma} \stackrel{L'H}{=} \frac{\varkappa}{1-\varkappa} \lim_{t \nearrow 1} \frac{(1 + (1-t)^\varkappa)^{-1} (1-t)^{\varkappa-1}}{(1-t)^{\gamma-1}} \\ &= \frac{\varkappa}{1-\varkappa} \lim_{t \nearrow 1} (1-t)^{\varkappa-\gamma} < \infty, \end{aligned}$$

Furthermore, the derivatives of η_{\varkappa} for $t \in (0, 1)$ are given by

$$\begin{aligned} \eta'_{\varkappa}(t) &= \frac{\varkappa}{1-\varkappa} \frac{t^{\varkappa-1} - (1-t)^{\varkappa-1}}{t^\varkappa + (1-t)^\varkappa}, \\ \eta''_{\varkappa}(t) &= \varkappa \frac{t^{\varkappa-2} + (1-t)^{\varkappa-2}}{t^\varkappa + (1-t)^\varkappa} - \frac{\varkappa^2}{1-\varkappa} \frac{(t^{\varkappa-1} + (1-t)^{\varkappa-1})^2}{(t^\varkappa + (1-t)^\varkappa)^2}. \end{aligned}$$

Thus we conclude that for $\varkappa < 1$:

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$$\begin{aligned}\eta'_\varkappa(t) &\simeq t^{\varkappa-1}, & \eta''_\varkappa(t) &\simeq t^{\varkappa-2}, & \text{for } t \searrow 0, \\ \eta'_\varkappa(t) &\simeq (1-t)^{\varkappa-1}, & \eta''_\varkappa(t) &\simeq (1-t)^{\varkappa-2}, & \text{for } t \nearrow 1,\end{aligned}$$

so that we may choose $\gamma \leq \varkappa$. For $1 < \varkappa \leq 2$ first note that the first derivatives in $t = 0$ and $t = 1$ are bounded but non-zero, so we have

$$\begin{aligned}\eta'_\varkappa(t) &\simeq 1, & \eta''_\varkappa(t) &\simeq t^{\varkappa-2}, & \text{for } t \searrow 0, \\ \eta'_\varkappa(t) &\simeq 1, & \eta''_\varkappa(t) &\simeq (1-t)^{\varkappa-2}, & \text{for } t \nearrow 1,\end{aligned}$$

and therefore we have to take $\gamma \leq 1$. Similarly for $\varkappa > 2$ we have

$$\begin{aligned}\eta'_\varkappa(t) &\simeq 1, & \eta''_\varkappa(t) &\simeq 1, & \text{for } t \searrow 0, \\ \eta'_\varkappa(t) &\simeq 1, & \eta''_\varkappa(t) &\simeq 1, & \text{for } t \nearrow 1,\end{aligned}$$

so we can only take $\gamma \leq 1$ as well. □

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