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The Fermionic Entanglement Entropy of the Vacuum State of a Schwarzschild Black Hole Horizon

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Abstract. We define and analyze the fermionic entanglement entropy of a Schwarzschild black hole horizon for the regularized vacuum state of an observer at infinity. Using separation of variables and an integral representation of the Dirac propagator, the entanglement entropy is computed to be a prefactor times the number of occupied angular momentum modes on the event horizon.

Contents

1. Introduction

Black hole thermodynamics is an exciting topic of current research in both physics and mathematics. It was initiated by the discovery of Bekenstein and Hawking that black holes behave thermally if one interprets surface gravity as temperature and the area of the event horizon as entropy [2,18]. The analogy to the second law of thermodynamics suggests that the area of the black hole horizon should only increase in time. However, this is in contradiction with the discovery of Hawking radiation and the resulting "evaporation" of a black hole [16,17]. This so-called *information paradox* [19] inspired the holographic principle [36,37] and the current program of attempting to understand the structure of spacetime via information theory, entropies and gauge/gravity dualities.

The present work is concerned with the entropy of a black hole. Generally speaking, *entropy* is a measure for the disorder of a physical system. There are various notions of entropy, like the entropy in classical statistical mechanics as introduced by Boltzmann and Gibbs, the Shannon and Rényi entropies in information theory or the von Neumann entropy for quantum systems. Here we focus on the *entanglement entropy*, which quantifies the quantum entanglement of a spatial region with its surrounding (for the general physical and mathematical context, see, for example, [21,29]). The entanglement entropy of the *event horizon* tells us about the quantum entanglement between the interior and exterior regions of the black hole. For technical simplicity, we here restrict attention to the simplest mathematical model of a black hole: a

Schwarzschild black hole of mass M (more general black holes will be discussed in the outlook section after (8.2)). We consider the *Rényi entropy* functional for a general Rényi parameter $\kappa > 0$. The case $\kappa = 1$ gives the *von Neumann entropy* functional. We compute the corresponding entanglement entropies for the *quasi-free fermionic state* describing the *vacuum* of an observer at infinity. More precisely, we consider the quasi-free fermionic Hadamard state which is obtained by frequency splitting for the observer in a rest frame in Schwarzschild coordinates, with an *ultraviolet regularization* on a length scale ε. In a more physical language, we consider a free Fermi gas formed of non-interacting one-particle Dirac states. Based on formulas derived in [20,25] (for more details, see the preliminaries in Sect. 2.1), the entanglement entropy can be expressed in terms of the reduced one-particle density operator. We choose this 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" refers to the Schwarzschild time of an observer at rest). Making use of the integral representation of the Dirac propagator in [8] and employing techniques developed in [25,32–34,39], it becomes possible to compute the entanglement entropy on the black hole horizon explicitly. 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 one-particle states. A similar result is obtained for the *Rényi entropies* with Rényi index $\kappa > \frac{2}{3}$.

We now outline our setting and the main result. The quasi-free regularized Dirac vacuum state can be described completely by the corresponding reduced one-particle density operator (for details see Sect. 2.1). We choose this operator as the regularized projection operator to the negative frequency solutions of the Dirac equation by Π_-^ε (for details see Sects. 3 and 4). Given a parameter $\kappa > 0$ (the *Rényi index*), we introduce the *Rényi entropy function* η_κ as follows. If $t \notin (0,1)$, then we set $\eta_\kappa(t) = 0$. For $t \in (0,1)$, we define

$$\eta_\kappa(t) = \frac{1}{1-\kappa} \log \left(t^\kappa + (1-t)^\kappa \right) \qquad \text{for } \kappa \neq 1 \qquad (1.1)$$

$$\eta_1(t) := \lim_{\kappa' \to 1} \eta_{\kappa'}(t) = -t \log t - (1-t) \log(1-t) \qquad \text{for } \kappa = 1 \qquad (1.2)$$

(the last limit can be computed directly with l'Hospital's rule). Note that the function η_κ is continuous and smooth except at $t = 0$ and $t = 1$, as shown in Fig. 1 for various values of κ. Note that η_1 is the familiar *von Neumann entropy function*. Next, we consider the *entropic difference operator* corresponding to the subset Λ as introduced [24, Section 3] (for more details and references, see the preliminaries in Sect. 2.1)

$$\Delta_\kappa(\Pi_-^\varepsilon, \Lambda) := \eta_\kappa\left(\chi_\Lambda \, \Pi_-^\varepsilon \, \chi_\Lambda \right) - \chi_\Lambda \, \eta_\kappa(\Pi_-^\varepsilon) \, \chi_\Lambda , \qquad (1.3)$$

In order to obtain the entropy of the event horizon, we choose Λ as an annular region around the event horizon. As the radial coordinate, we choose Regge–Wheeler coordinate $u \in \mathbb{R}$, in which the event horizon is located at $u \to -\infty$
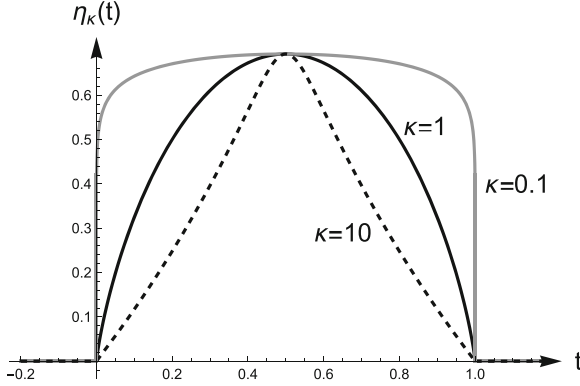
FIGURE 1. Plot of the function η_κ for $\kappa = 0.1$, 1 and 10

(for details, see (2.5) in the preliminaries). We then parametrize Λ by

$$\Lambda := \mathcal{K} \times S^2 \qquad \text{with} \qquad \mathcal{K} := (u_0 - \rho, u_0)$$

$$\equiv \left\{ \begin{pmatrix} u \sin \vartheta \cos \varphi \\ u \sin \vartheta \sin \phi \\ u \cos \vartheta \end{pmatrix} \ \middle| \ u_0 - \rho < u < u_0, \ 0 < \vartheta < \pi, \ 0 < \varphi < 2\pi \right\} \quad (1.4)$$

(see also Fig. 2 on page 29). The *fermionic entanglement entropy* is obtained as the trace of the entropic difference operator (1.3) in the limit when Λ moves toward the event horizon, i.e.,

$$S_\kappa(\Pi_-^\varepsilon, \Lambda) := \lim_{u_0 \to -\infty} \operatorname{tr} \left(\Delta_\kappa(\Pi_-^\varepsilon, \Lambda) \right). \qquad (1.5)$$

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 $u_0 \to -\infty$. 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. For ease in presentation, we begin with one angular momentum mode parametrized by (k, n) with $k \in \mathbb{Z} + 1/2$ and $n \in \mathbb{N}$ (for details on the separation of variables of the Dirac equation, see the preliminaries in Sect. 2.3). Then the trace in (1.5) becomes

$$\operatorname{tr} \Delta_\kappa \left((\Pi_-^\varepsilon)_{kn}, \mathcal{K} \right),$$

where $(\Pi_-^\varepsilon)_{kn}$ is the operator Π_ε^i restricted to the angular mode (k, n). This operator depends only on the radial variable; this is why the characteristic function χ_Λ has been replaced by $\chi_\mathcal{K}$. We define the *mode-wise Rényi entropy* of the black hole as

$$S_{\kappa, kn}^{\mathrm{BH}} := \frac{1}{2} \lim_{\rho \to \infty} \lim_{\varepsilon \searrow 0} \frac{1}{f(\varepsilon)} \lim_{u_0 \to -\infty} \operatorname{tr} \Delta_\kappa \left((\Pi_-^\varepsilon)_{kn}, \mathcal{K} \right), \qquad (1.6)$$

where $f(\varepsilon)$ is a function describing the highest order of divergence in ε (we will later see that here $f(\varepsilon) = \log(M/\varepsilon)$ with M the black hole mass). Our main result shows that $S^{\mathrm{BH}}_{\kappa,kn}$ has the same numerical value for each angular mode:

Theorem 1.1. *Let $\kappa > \frac{2}{3}$ and let $n \in \mathbb{Z}$ and $k \in \mathbb{Z} + 1/2$ arbitrary, then*

$$\lim_{\varepsilon \searrow 0} \lim_{u_0 \to -\infty} \frac{1}{\log(\ell/\varepsilon)} \operatorname{tr} \Delta_\kappa \big((\Pi^\varepsilon_-)_{kn}, \mathcal{K}\big) = \frac{1}{12} \frac{\kappa + 1}{\kappa} , \qquad (1.7)$$

where ℓ is a reference length. Due to the form of the Rényi entropy functions, the right-hand side is always positive. For the entanglement entropy, i.e., $\kappa = 1$, we obtain in particular

$$\lim_{\varepsilon \searrow 0} \lim_{u_0 \to -\infty} \frac{1}{\log(\ell/\varepsilon)} \operatorname{tr} \Delta_1 \big((\Pi^\varepsilon_-)_{kn}, \mathcal{K}\big) = \frac{1}{6} . \qquad (1.8)$$

We note for clarity that the only purpose of the reference length ℓ is to make the argument of the logarithm dimensionless. The choice of ℓ is irrelevant, because writing $\log(\ell/\varepsilon) = \log \ell - \varepsilon$, the term $\log \ell$ is sub-leading. Thus, the main statement of (1.7) and (1.8) is that, in the limit $\varepsilon \searrow 0$, the traces are logarithmically divergent, and we determine the corresponding proportionality factor. Since the mass of the Dirac particles will be irrelevant, it is natural to associate ℓ with the only other parameter with dimension of length: the mass M of the black hole. Therefore, in what follows we will always replace the logarithm in the above formulas by $\log(M/\varepsilon)$ (for more on units, see the last paragraph of introduction).

In simple terms, the above result shows that each occupied angular momentum mode gives the same contribution to the (Rényi) entanglement entropy. This result can be understood immediately from the infinite red shift effect at the event horizon. Indeed, asymptotically near the event horizon, a Dirac wave behaves like a massless particle without angular momentum (as will be made precise in Lemma 2.3), suggesting that also the entanglement entropy should be the same for each angular mode. Proving this result, however, makes it necessary to estimate different error terms, which constitutes the technical core of this work.

The (Rényi) entanglement entropy of the black hole can be written formally as the sum of all angular momentum modes,

$$S^{\mathrm{BH}}_\kappa = \sum_{k,n} S^{\mathrm{BH}}_{\kappa,kn} . \qquad (1.9)$$

Since each angular mode gives the same non-zero contribution (1.8), the sum in (1.9) clearly diverges if an infinite number of angular modes are occupied. This leads us to regularize the vacuum state by also occupying only a finite number of angular momentum modes (for details see (4.2) in Sect. 4). After this has been done, the sum in (1.9) becomes finite. Then, applying Theorem 1.1 to each angular mode, it becomes 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 [35] and

loop quantum gravity [1]. In order to push the analogy further, assuming a minimal area ε^2 on the horizon and keeping in mind that the area of the event horizon scales like M^2 (as is obvious already from dimensional considerations), 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. The factor $\log(M/\varepsilon)$ in the above theorem is usually referred to as an *enhanced* area law. Such an enhanced area law typically occurs if the considered fields are massless, in which case long-range effects give rise to an additional logarithmic divergence. This fits to our physical situation because, as mentioned above, the Dirac wave behaves near the event horizon like as massless field due to the red shift effect at the event horizon. We also note for clarity that we make essential use of the fact that our vacuum state involves a hard cutoff between the occupied one-particle states of negative frequency and the non-occupied states of positive frequency. It is not clear to us if considering instead a smooth cutoff function would still lead to an enhanced area law.

The article is structured as follows. Section 2 provides the necessary preliminaries on entanglement entropy, the Dirac equation, the Dirac propagator in the Schwarzschild geometry and some technical tools involving Schatten classes and pseudo-differential operators. In Sect. 3, the regularized projection operator on 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 in the language of pseudo-differential operators. Moreover, the symbol will be further simplified at the horizon. After these preparations, the core of this works begins in Sect. 4, where the regularized fermionic vacuum and the corresponding (Rényi) entanglement entropy of the event horizon are defined. In Sect. 5, there is the entropy of a simplified limiting operator (in the sense that the regularization goes to zero) at the horizon. Afterward, we estimate the error caused by using the limiting operator instead of the regularized one (Sect. 6). It turns out that this error drops out in the limiting process. Subsequently, we complete the proof of the main result (Theorem 1.1) by combining the results from the previous sections (Sect. 7). We conclude with a brief summary and a discussion of open problems (Sect. 8). The appendices contain additional material and give some background information.

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

$$\text{dimensionless quantities} \qquad m\ell\,, \quad \frac{M}{\ell} \quad \text{and} \quad \frac{\varepsilon}{\ell} \qquad (1.10)$$

(where m is the mass of the Dirac particles, M is the mass of the black hole times the gravitational constant and ε is the regularization length). 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 geometry, it is natural to choose ℓ as the black hole mass M.

We conclude the introduction with some general notational conventions. 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.

For any vector space V, we denote
$$\mathrm{L}(V) := \{ f : V \to V \mid f \text{ bounded and linear} \}.$$

Finally, for ease of notation the operator of multiplication by f is denoted with the same letter, i.e., $(f\psi)(x) := f(x)\,\psi(x)$.

2. Preliminaries

2.1. The Entanglement Entropy of a Quasi-Free Fermionic State

Given a Hilbert space $(\mathcal{H}_m, \langle.|.\rangle_m)$ (the "one-particle Hilbert space"), we let $(\mathcal{F}, \langle.|.\rangle_\mathcal{F})$ be the corresponding fermionic Fock space, i.e.,
$$\mathcal{F} = \bigoplus_{k=0}^{\infty} \underbrace{\mathcal{H}_m \wedge \cdots \wedge \mathcal{H}_m}_{k \text{ factors}}$$
(where $\wedge$ denotes the totally anti-symmetrized tensor product). We define the *creation operator* $\Psi^\dagger$ by
$$\Psi^\dagger \,:\, \mathcal{H}_m \to \mathrm{L}(\mathcal{F}), \qquad \Psi^\dagger(\psi)(\psi_1 \wedge \cdots \wedge \psi_p) := \psi \wedge \psi_1 \wedge \cdots \wedge \psi_p.$$
Its adjoint is the annihilation operator denoted by $\Psi(\overline{\psi}) := (\Psi^\dagger(\psi))^*$. These operators satisfy the canonical anti-commutation relations
$$\{\Psi(\overline{\psi}), \Psi^\dagger(\phi)\} = (\psi|\phi) \qquad \text{and} \qquad \{\Psi(\overline{\psi}), \Psi(\overline{\phi})\} = 0 = \{\Psi^\dagger(\psi), \Psi^\dagger(\phi)\}.$$
Next, we let W be a *statistical operator* on $\mathcal{F}$, i.e., a positive semi-definite linear operator of trace one,
$$W \,:\, \mathcal{F} \to \mathcal{F}, \qquad W \geq 0 \quad \text{and} \quad \mathrm{tr}_\mathcal{F}(W) = 1.$$
Given an observable A (i.e., a symmetric operator on $\mathcal{F}$), the expectation value of the measurement is given by
$$\langle A \rangle := \mathrm{tr}_\mathcal{F}\left(AW\right).$$
The corresponding *quantum state* Ω is the linear functional which to every observable associates the expectation value, i.e.,
$$\Omega \,:\, A \mapsto \mathrm{tr}_\mathcal{F}\left(AW\right).$$

In this work, we restrict our attention to the subclass of so-called *quasi-free* quantum states, fully determined by their two-point functions
$$\Omega_2(\overline{\psi}, \phi) := \Omega\big(\Psi^\dagger(\phi)\,\Psi(\overline{\psi})\big), \qquad \text{for any } \psi, \phi \in \mathcal{H}_m.$$

Definition 2.1. The **reduced one-particle density operator** D is the positive linear operator on the Hilbert space $(\mathcal{H}_m, (.|.)_{\mathcal{M}})$ defined by

$$\Omega_2(\overline{\psi}, \phi) = \langle \psi \,|\, D\phi \rangle_m \,, \qquad \text{for any } \psi, \phi \in \mathcal{H}_m \,.$$

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

$$S(\Omega) = \operatorname{tr} \eta_1(D) \,, \tag{2.1}$$

where η_κ is the function from (1.2) (for a plot, see Fig. 1). This formula appears commonly in the literature (see, for example, [28, Equation 6.3], [7, 22, 26] and [20, eq. (34)]). A detailed derivation is found in [11, Appendix A]. Similar to (2.1) also other entropies can be expressed in terms of the reduced one-particle density operator. In particular, the Rényi entropy can be written as $S_\kappa(\Omega) = \operatorname{tr} \eta_\kappa(D)$ This formula is also derived in [11, Appendix A].

For the *entanglement entropy*, we need to assume that the Hilbert space $\mathcal{H}_m$ is formed of wave functions in spacetime. Restricting them to a Cauchy surface, we obtain functions defined on three-dimensional space $\mathcal{N}$ (which could be $\mathbb{R}^3$ or, more generally, a three-dimensional manifold). Given a spatial subregion $\Lambda \subset \mathcal{N}$, we define the (Rényi) entanglement entropy by

$$S_\kappa(D, \Lambda) := \operatorname{tr} \left(\eta_\kappa\big(\chi_\Lambda\, D\, \chi_\Lambda\big) - \chi_\Lambda\, \eta_\kappa(D)\, \chi_\Lambda \right) . \tag{2.2}$$

More details in the case $\kappa = 1$ can be found in [24, Section 3].

2.2. The Dirac Equation in Globally Hyperbolic Spacetimes

Since we are ultimately interested in Schwarzschild space time, the abstract setting for the Dirac equation is given as follows (for more details see, for example, [12]). 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 fibers $S_x\mathcal{M}$ are endowed with an inner product $\prec.|.\succ_x$ of signature $(2, 2)$, referred to as the spin inner product. Moreover, the mapping

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

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, $C_0^\infty(\mathcal{M}, S\mathcal{M})$ 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

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

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

$$(\mathcal{D} - m)\, \psi = 0 \,. \tag{2.3}$$

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 $C_{\mathrm{sc}}^\infty(\mathcal{M}, S\mathcal{M})$. The solutions in this class are endowed with the scalar product

$$(\psi|\phi)_m = \int_{\mathcal{N}} \prec\!\psi \,|\, \nu^j \gamma_j \, \phi\!\succ_x \mathrm{d}\mu_{\mathcal{N}}(x) \,, \qquad (2.4)$$

where $\mathcal{N}$ is a Cauchy surface $\mathcal{N}$ with future-directed normal ν and $\mathrm{d}\mu_{\mathcal{N}}$ denotes the measure on $\mathcal{N}$ induced by the metric g (compared to the conventions in [12], we here preferred to leave out a factor of 2π). This scalar product is independent of the choice of $\mathcal{N}$ (for details see [12, Section 2]). Finally, we define the Hilbert space $(\mathcal{H}_m, (.|.)_m)$ by completion,

$$\mathcal{H}_m := \overline{C_{\mathrm{sc}}^\infty(\mathcal{M}, S\mathcal{M})}^{(.|.)_m} \,.$$

2.3. The Dirac Propagator in the Schwarzschild Geometry

2.3.1. 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 [8] and [14]. Given a parameter $M > 0$ (the black hole mass), the exterior Schwarzschild metric reads

$$\mathrm{d}s^2 = g_{jk} \, \mathrm{d}x^j \, \mathrm{d}x^k = \frac{\Delta(r)}{r^2} \, \mathrm{d}t^2 - \frac{r^2}{\Delta(r)} \, \mathrm{d}r^2 - r^2 \, \mathrm{d}\vartheta^2 - r^2 \, \sin^2\vartheta \, \mathrm{d}\varphi^2 \,,$$

where

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

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

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

where $r_1 := 2M$ is the event horizon. It is most convenient to transform the radial coordinate to the so called *Regge–Wheeler coordinate* $u \in \mathbb{R}$ defined by

$$u(r) = r + 2M \log(r - 2M) \,, \qquad \text{so that} \qquad \frac{\mathrm{d}u}{\mathrm{d}r} = \frac{r^2}{\Delta(r)} \,. \qquad (2.5)$$

In this coordinate, the event horizon is located at $u \to -\infty$, whereas $u \to \infty$ corresponds to spatial infinity, i.e., $r \to \infty$.

In this geometry, the Dirac operator takes the form (see also [14, Section 2.2]):

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

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

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

Then the Dirac equation can be separated with the ansatz

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

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 $L^2\big(((-1,1),\, d\vartheta\cos\vartheta),\mathbb{C}^2\big)$ (see [14, Section 2.4] with additional reference to [15]). The radial functions $X_{\pm}^{kn}$ satisfy a system of partial differential equations

$$\begin{pmatrix} \sqrt{\Delta(r)}\,\mathcal{D}_+ & imr - \lambda \\ -imr - \lambda & \sqrt{\Delta(r)}\,\mathcal{D}_- \end{pmatrix} \begin{pmatrix} X_+^{kn} \\ X_-^{kn} \end{pmatrix} = 0 \,, \tag{2.6}$$

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 [8, Section 2]. Moreover, employing the ansatz

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

equation (2.6) 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 $X_a^{kn\omega} = (X_{a,+}^{kn\omega}, X_{a,-}^{kn\omega})$. In the case $|\omega| < m$, these solutions behave exponentially near infinity. We always choose the fundamental solution for

$$a = 1 \text{ as the fundamental solution which } decays \text{ at infinity.} \tag{2.7}$$

For more details on the choice of the fundamental solutions, see Sect. 2.3.4.

In what follows, we will often use the following notation for two-component functions

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

The norm in $\mathbb{C}^2$ will be denoted by $|.|$, the canonical inner product on $L^2(\mathbb{R},\mathbb{C}^2)$ by $\langle . | . \rangle$ and the corresponding norm by $\|.\|$.

As implied by [8, Theorem 3.6], one can then find the following formula for the mode-wise propagator:

Theorem 2.2. *Given initial radial data $X_0 \in C_0^\infty(\mathbb{R},\mathbb{C}^2)$ at time $t = 0$, the corresponding solution $X \in C^\infty(\mathbb{R}^2,\mathbb{C}^2)$ of the radial Dirac equation (2.6) can be written as*

$$X(t,u) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega\, e^{-i\omega t} \sum_{a,b=1}^{2} t_{ab}^{kn\omega}\, X_a^{kn\omega}(u)\, \langle X_b^{kn\omega}|X_0\rangle \,, \tag{2.8}$$

for any $t, u \in \mathbb{R}$. The $X_a^{kn\omega}(x)$ 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

$$\begin{cases} t_{ab}^{kn\omega} = \delta_{a,1}\,\delta_{b,1} & \text{if } |\omega| \leq m \\ t_{11}^{kn\omega} = t_{22} = \dfrac{1}{2}\,, \quad \left|t_{12}^{kn\omega}\right| \leq \dfrac{1}{2} & \text{if } |\omega| > m\,. \end{cases} \tag{2.9}$$

We note for clarity that, in view of (2.9) and (2.7), in the case $|\omega| < m$ only the exponentially decaying wave function enters the integral representation. This has the effect that, asymptotically near infinity, only the spectrum for $|\omega| \geq m$ is visible, in agreement with the mass gap in Minkowski space.

2.3.2. Hamiltonian Formulation. The Dirac equation (2.3) can be written in the Hamiltonian form

$$i\partial_t \psi = H\psi\,, \tag{2.10}$$

where the Hamiltonian H is a spatial operator acting on the spinors. Choosing the Cauchy surface $\mathcal{N}$ as the surface of constant Schwarzschild time and the domain $\mathcal{D}(H)$ as the smooth and compactly supported spinorial wave functions on $\mathcal{N}$, the Hamiltonian is symmetric with respect to the scalar product (2.4), i.e.,

$$(H\psi \,|\, \phi)_m = (\psi \,|\, H\phi)_m \qquad \text{for all } \psi, \phi \in \mathcal{D}(H)$$

(for more details on this point in general stationary spacetimes, see [9, Section 4.6]). The Hamiltonian is essentially self-adjoint (see [13] for details in a more general context). Denoting the unique self-adjoint extension again by H, the Cauchy problem can be solved with the spectral calculus by

$$\psi(t) = e^{-itH}\,\psi_0\,. \tag{2.11}$$

This is the abstract counterpart of the integral representation of Theorem 2.2. In simple terms, the solution (2.8) can be understood as giving an integral representation for the operator e^{-itH} restricted to an angular mode. Noting that ω is the spectral parameter, the integral in (2.8) can be understood as a spectral decomposition in terms of the spectral measure (in particular, the spectrum of the Hamiltonian is the whole real axis). In order to make these connections more precise, we first note that also the radial Dirac equation after separation of variables (2.6) can be written in the Hamiltonian form

$$i\frac{\partial}{\partial t}X^{kn}(t,u) = \left(H_{kn}X^{kn}|_t\right)(u)$$

$$\iff \quad (\mathcal{D} - m)\,e^{-ik\varphi}\,\frac{1}{\Delta(r)^{1/4}\sqrt{r}}\begin{pmatrix} X_-^{kn}(t,u)Y_-^{kn}(\vartheta) \\ X_+^{kn}(t,u)Y_+^{kn}(\vartheta) \\ X_+^{kn}(t,u)Y_-^{kn}(\vartheta) \\ X_-^{kn}(t,u)Y_+^{kn}(\vartheta) \end{pmatrix} = 0\,,$$

where the Hamiltonian H_{kn} now is an essentially self-adjoint operator on $L^2(\mathbb{R}, \mathbb{C}^2)$ with dense domain $\mathcal{D}(H_{kn}) = C_0^\infty(\mathbb{R}, \mathbb{C}^2)$. This makes it possible to write the solution of the Cauchy problem as

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

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., $X_0 \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$, then the time evolution operator can be written with the help of Theorem 2.2 as

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

$$\text{for } X_0 \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$$

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 work.

2.3.3. Connection to the Full Propagator. We now explain how the solution of the Cauchy problem as given abstractly in (2.11) can be decomposed into angular modes. Our considerations explain why we may restrict attention to one angular mode instead of the full propagator and why we can use the ordinary L^2-scalar product instead of $(.|.)_m$. We introduce the function

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

Moreover, for each fixed $k \in \mathbb{Z} + 1/2$ and $n \in \mathbb{Z}$ we denote by $(\mathcal{H}_m^0)_{kn}$ the completion of the vector space

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

with respect to the scalar product $(.|.)_m$ introduced in (2.4), i.e.,

$$(\mathcal{H}_m^0)_{kn} := \overline{V_{kn}}^{(.|.)_m}.$$

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

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

has the orthogonal decomposition

$$\mathcal{H}_m^0 = \bigoplus_{i \in \mathbb{N}} (\mathcal{H}_m^0)_{k_i n_i}. \tag{2.12}$$

(again with respect to $(.|.)_m$), where $((k_i, n_i))_{i \in \mathbb{N}}$ is an enumeration of $(\mathbb{Z} + 1/2) \times \mathbb{Z}$. Furthermore, each space $(\mathcal{H}_m^0)_{kn}$ can be connected with $L^2(\mathbb{R}, \mathbb{C}^2)$ using the mapping

$$\tilde{S} : \left((\mathcal{H}_m^0)_{kn}, \, (.|.)\right) \to L^2(\mathbb{R}, \mathbb{C}^2),$$

which for any $(\psi_1, \cdots, \psi_4) \in (\mathcal{H}_m^0)_{kn}$ is given by

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

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

It has the inverse

$$
\tilde{S}^{-1} : L^2(\mathbb{R}, \mathbb{C}^2) \to \big((\mathcal{H}_m^0)_{kn}, \, (.|.)_m\big),
$$

$$
(X_+, X_-) \mapsto S^{-1} e^{-ik\varphi} \begin{pmatrix} X_-(u) Y_-^{kn}(\vartheta) \\ X_+(u) Y_+^{kn}(\vartheta) \\ X_+(u) Y_-^{kn}(\vartheta) \\ X_-(u) Y_+^{kn}(\vartheta) \end{pmatrix}.
$$

Then a direct computation shows the scalar products transform as

$$
\langle \tilde{S}\psi \,|\, \tilde{S}\phi \rangle_{L^2} = (\psi \,|\, \phi)_m \qquad \text{for any } \phi, \psi \in (\mathcal{H}_m^0)_{kn}.
$$

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 (2.12))

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

defines an essentially self-adjoint Hamiltonian for the original Dirac equation on the space $\mathcal{H}_m^0$.

Moreover, any function of $\tilde{H}$ is of the same diagonal block operator form. The same holds for any multiplication operator $\mathcal{M}_{\chi_{\tilde{U}}}$, 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

$$
\mathcal{M}_{\chi_{\tilde{U}}} = \mathrm{diag}\big(\mathcal{M}_{\chi_{\tilde{U}}}, \, \mathcal{M}_{\chi_{\tilde{U}}}, \, \dots \big).
$$

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

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

(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 $(\mathcal{H}^0_m)_{kn}$ 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 $\mathcal{M}_{\chi_{\tilde{U}}}$ goes over to $\mathcal{M}_{\chi_U}$, i.e.,

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

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

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

2.3.4. 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 solutions $X^{kn\omega}$. In order to control the resulting error terms, we now state a slightly stronger version of [8, Lemma 3.1], specialized to the Schwarzschild case.

Lemma 2.3. *For any $u_2 \in \mathbb{R}$ fixed, in Schwarzschild space every solution $X \equiv X^{kn\omega}$ for $u \in (-\infty, u_2)$ is of the form*

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

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

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

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

$$|g(u)| < c e^{du} , \qquad \left| \frac{\mathrm{d}}{\mathrm{d}u} g(u) \right| \le dc e^{du} \qquad \text{for all } u < u_2 ,$$

with coefficients $c, d > 0$ that can be chosen independently of ω and $u < u_2$.

The proof, which follows the method in [8], is given in detail in Appendix B.

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 [8, p. 41] and [14, p. 9–10]). In the case $|\omega| > m$, we choose X_1 and X_2 such that the corresponding functions f_0 from the previous lemma are of the form

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

In the case $|\omega| \le m$, we consider the behavior of solutions at infinity (i.e., asymptotically as $u \to \infty$). 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

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

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

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

Note, however, that f_0 and R_0 from the previous lemma may in general also depend on k and n, but for ease in notation this dependence will be suppressed.

2.4. A Few Functional Analytic Tools

2.4.1. Basic Definitions. Later will often rewrite operators on $L^2(\mathbb{R}^d, \mathbb{C}^n)$ as pseudo-differential operators of the form

$$\left(\mathrm{Op}_\alpha(\mathcal{A}) \psi \right)(\boldsymbol{x}) := \left(\frac{\alpha}{2\pi} \right)^d \int_{\mathbb{R}^d} \int_{\mathcal{U}} e^{-i\alpha \boldsymbol{\xi} \cdot (\boldsymbol{x} - \boldsymbol{y})} \, \mathcal{A}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\xi}) \, \psi(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} \, \mathrm{d}\boldsymbol{\xi} \tag{2.13}$$
$$\text{for any } \psi \in C_0^\infty(\mathcal{U}, \mathbb{C}^n) \ .$$

where $\mathcal{U} \subseteq \mathbb{R}^d$ is some open set. The so-called *symbol* $\mathcal{A}$ is a suitable measurable matrix-valued map $\mathcal{A} : (\mathbb{R}^d)^3 \times (0, \infty) \to \mathrm{M}(n, n)$ such that the operator on $C_0^\infty(\mathcal{U}, \mathbb{C}^n)$ defined by (2.13) can be extended continuously to all of $L^2(\mathcal{U}, \mathbb{C}^n)$. 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 if $\mathcal{U} \subsetneq \mathbb{R}^d$, then the operator $\mathrm{Op}_\alpha(\mathcal{A})$ may still be considered an operator on $L^2(\mathbb{R}^d, \mathbb{C}^n)$ if one replaces $\mathcal{A}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\xi})$ by $\chi_\mathcal{U}(\boldsymbol{x}) \mathcal{A}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\xi}) \chi_\mathcal{U}(\boldsymbol{y})$. In fact in what follows, we often identify these operators. Symbols denoted by lowercase letters usually indicate that the symbol is scalar valued. Moreover, the symbols sometimes additionally depend on α or other parameters. We usually denote this by corresponding super- or subscripts. For some symbols $\mathcal{A}$, the integral representation (2.13) extends to all Schwartz or even all L^2-functions. If this condition is needed for specific results, we will mention it explicitly. We will also establish some conditions on $\mathcal{A}$ that guarantee such extensions. The names of the arguments of the symbol $\mathcal{A}$ are adapted to the application in mind. In particular, if symbols that are *not* boldface, this usually implies that they are scalar valued, i.e., $d = 1$.

In order to conveniently compute the entanglement entropy, we will often be interested in the trace of the following operator:

$$D_\alpha(\eta_\kappa, \Lambda, \mathcal{A}) := \eta_\kappa \big(\chi_\Lambda \mathrm{Op}_\alpha(\mathcal{A}) \chi_\Lambda \big) - \chi_\Lambda \eta_\kappa \big(\mathrm{Op}_\alpha(\mathcal{A}) \big) \chi_\Lambda \ ,$$

where $\Lambda \subseteq \mathbb{R}^d$ is some measurable set which will be specified later.

Moreover, in what follows we will often use the notation

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

for some measurable set $\Omega \subseteq \mathbb{R}^d$, which emphasizes that this is a projection operator (that it is well defined follows from Lemma A.1 in Appendix A). In Remark A.2, we will see that the integral representation of such operators always extends to all Schwartz functions.

Furthermore, as we will later see, we can often estimate traces of functions of operators in terms of *Schatten norms*, which we now introduce (we refer to [5, Ch. 11] for more details on this topic). For a compact operator A in a separable Hilbert space $\mathfrak{H}$, we denote by $s_k(A), k = 1, 2, \ldots$, its singular values, i.e., eigenvalues of the self-adjoint compact operator $\sqrt{A^*A}$ labeled in non-increasing-order counting multiplicities. For the sum $A + B$, the following inequality holds:

$$s_{2k}(A + B) \le s_{2k-1}(A + B) \le s_k(A) + s_k(B). \tag{2.14}$$

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

$$\|A\|_p := \left(\operatorname{tr}(A^*A)^{\frac{p}{2}} \right)^{\frac{1}{p}}$$

is finite. The functional $\|A\|_p$ defines a norm if $p \ge 1$ and a quasi-norm if $0 < p < 1$. With this (quasi-)norm, the class $\mathfrak{S}_p$ is a complete space. For $0 < p \le 1$, the quasi-norm is actually a *p-norm*, that is, it satisfies the following triangle inequality for all $A, B \in \mathfrak{S}_p$,

$$\|A + B\|_p^p \le \|A\|_p^p + \|B\|_p^p \qquad (0 < p \le 1). \tag{2.15}$$

Moreover, for all $A \in \mathfrak{S}_{q_1}$ and $B \in \mathfrak{S}_{q_2}$ the following Hölder-type inequality holds (see [33, Section 2.1] with reference to [5, p. 262]),

$$\|AB\|_q \le \|A\|_{q_1} \|B\|_{q_2}, \qquad \text{with } q^{-1} = q_1^{-1} + q_2^{-1}, \quad 0 < q_1, q_2 \le \infty. \tag{2.16}$$

Remark 2.4. We note that the q-th Schatten norm is invariant under unitary transformations: Let $\mathfrak{H}$ and $\mathfrak{G}$ be Hilbert spaces, $U \in \mathrm{L}(\mathfrak{G}, \mathfrak{H})$ unitary and $A \in \mathfrak{S}^q \subseteq \mathrm{L}(\mathfrak{H})$, then

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

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

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

In particular, in the case $q = 1$ this shows that the trace norm of A is conserved under unitary transformation. ◇

Moreover, we will frequently use the following function norms (see, for example, [32, p. 5–6] with slight modifications)

Definition 2.5. Let $S^{(n,m,k)}(\mathbb{R}^d)$ with $m, n, k \in \mathbb{N}_0$ 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 n, in the second to m

and in the third to k and whose partial derivatives up to these orders are bounded as well. For $a \in S^{(n,m,k)}(\mathbb{R}^d)$ and $l, r > 0$, we introduce the norm

$$N^{(n,m,k)}(a; l, r) := \max_{\substack{0 \le \tilde{n} \le n \\ 0 \le \tilde{m} \le m \\ 0 \le \tilde{k} \le k}} \sup_{\bm{x}, \bm{y}, \bm{\xi}} l^{\tilde{n}+\tilde{m}} r^{\tilde{k}} \big| \nabla_{\bm{x}}^{\tilde{n}} \nabla_{\bm{y}}^{\tilde{m}} \nabla_{\bm{\xi}}^{\tilde{k}} a(\bm{x}, \bm{y}, \bm{\xi}) \big| \, .$$

Similarly, $S^{(n,k)}(\mathbb{R}^d)$ with $n, k \in \mathbb{N}_0$ denotes the space of all complex-valued functions on $(\mathbb{R}^d)^2$, which are continuous and bounded and continuously partially differentiable in the first variable up to order n and in the second to k and whose partial derivatives up to these orders are bounded. For $a \in S^{(n,m)}(\mathbb{R}^d)$ and $l, r > 0$, we introduce the norm

$$N^{(n,k)}(a; l, r) := \max_{\substack{0 \le \tilde{n} \le n \\ 0 \le \tilde{k} \le k}} \sup_{\bm{x}, \bm{\xi}} l^{\tilde{n}} r^{\tilde{k}} \big| \nabla_{\bm{x}}^{\tilde{n}} \nabla_{\bm{\xi}}^{\tilde{k}} a(\bm{x}, \bm{\xi}) \big| \, .$$

Finally, by $S^{(k)}(\mathbb{R}^d)$ with $k \in \mathbb{N}_0$ 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 k and whose partial derivatives up to these orders are bounded. For $a \in S^{(k)}(\mathbb{R}^d)$ and $r > 0$, we introduce the norm

$$N^{(k)}(a; r) := \max_{0 \le \tilde{k} \le k} \sup_{\bm{\xi}} r^{\tilde{k}} \big| \nabla_{\bm{\xi}}^{\tilde{k}} a(\bm{\xi}) \big| \, .$$

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

$$a(\bm{x}, \bm{y}, \bm{\xi}) \equiv a(\bm{x}, \bm{\xi}) \qquad \text{for all } \bm{y} \in \mathbb{R}^d \, .$$

Then, for any $l, r > 0$ one has

$$N^{(n,m,k)}(a; l, r) = N^{(n,k)}(a; l, r) \, .$$

2.4.2. Estimates on q-Normed Ideals. In order to generalize a theorem by Widom (Theorem 5.3) later on, we need a few estimates, which we state here. Since Theorem 5.3 admits only smooth functions, the next two lemmata will allow us to extend it to certain functions which do not need to be differentiable everywhere.

Lemma 2.6 [34, Cor. 2.11, Cond. 2.9, Thm. 2.10]. *Let $q, r > 0$ parameters, $n \ge 2$ a natural number and $f \in C_0^n(-r, r)$. Let $\mathfrak{S} \subset L(\mathfrak{H})$ (with a Hilbert space $\mathfrak{H}$) be a q-normed ideal such that there is $\sigma \in (0, 1]$ with*

$$(n - \sigma)^{-1} < q \le 1 \, .$$

Moreover, consider a self-adjoint operator A on $D(A) \subseteq \mathfrak{H}$ and a projection operator P such that $PD(A) \subseteq D(A)$ and $|PA(\mathbb{1} - P)|^\sigma \in \mathfrak{S}$ and $PA(\mathbb{1} - P)$ extends to a bounded operator. Then

$$\|f(PAP)P - Pf(A)\|_{\mathfrak{S}} \lesssim \max_{0 \le k \le n} \left(r^k \|f^{(k)}\|_{L^\infty} \right) r^{-\sigma} \left\| |PA(\mathbb{1} - P)|^\sigma \right\|_{\mathfrak{S}}$$

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

We will usually apply this and the following lemma to operators of the form

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

for some subset $\Lambda \subseteq \mathbb{R}^d$ and with $\mathfrak{S}$ as the qth Schatten class.

In preparation for the next lemma, we introduce the following condition.

Condition 2.7 [34, Condition 2.3]. *Let $n \in \mathbb{N}$ and $f \in C^n(\mathbb{R}\backslash\{t_0\}) \cap C(\mathbb{R})$ a function with $t_0 \in \mathbb{R}$, such that there exist $\gamma, R > 0$ with*

$$\big\| f \big\|_n := \max_{0 \le k \le n} \sup_{t \ne t_0} |f^{(k)}(t)| \cdot |t - t_0|^{-\gamma + k} < \infty \,, \tag{2.17}$$

and $\mathrm{supp}\, f \subseteq [t_0 - R, t_0 + R]$.

Lemma 2.8 [34, Theorem 2.10]. *Let f satisfy Condition 2.7 for some $n \ge 2$ and $\gamma, R > 0$. Let $\mathfrak{S}$, A and P as in Lemma 2.6 with $\sigma < \gamma$, then*

$$\big\| f(PAP)P - Pf(A) \big\|_{\mathfrak{S}} \lesssim \big\| f \big\|_n R^{\gamma - \sigma} \big\| |PA(\mathbb{1} - P)|^\sigma \big\|_{\mathfrak{S}} \,,$$

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

Example 2.9. Ultimately we want to apply Lemma 2.8 to η_κ (times a cutoff function). Therefore, we introduce the function

$$f(x) := \eta_\kappa(x)\, \Phi_1(x) \,, \qquad \text{for any } x \in \mathbb{R} \,,$$

with a smooth non-negative function Φ_1 such that

$$\mathrm{supp}\, \Phi_1 = \left[-\frac{3}{4}, \frac{3}{4} \right] \qquad \text{and} \qquad \Phi_1\big|_{\left[-\frac{1}{2}, \frac{1}{2}\right]} \equiv 1 \,.$$

Note that f then satisfies the conditions of Lemma 2.8 for any $n \in \mathbb{N}$, $\gamma < 1$ arbitrary, $R = 3/4$ and $x_0 = 0$.

This gives an idea how Lemma 2.8 can be used to estimate the error in Theorem 5.3 caused by functions like η_κ, which are not differentiable everywhere. ◇

2.4.3. Estimates of Pseudo-Differential Operators. Here we list a few previously establishes estimates on pseudo-differential operators, which we will use later on. The first lemma shows that $\mathrm{Op}_\alpha(a)$ is bounded with respect to the operator norm uniformly in α as long as $a \in S^{(n,m,k)}(\mathbb{R}^d)$.

Lemma 2.10 [32, Lemma 3.9] (adapted to our notation). *Let $a \in S^{(k,k,d+1)}(\mathbb{R}^d)$ be a symbol such that $\mathrm{Op}_\alpha(a)$ is well defined and its integral representation extends to all Schwartz functions. We choose $k := \lfloor d/2 \rfloor + 1$, $l_0 > 0$ and $l, r > 0$ such that $\alpha l r \ge l_0$. Then*

$$\|\mathrm{Op}_\alpha(a)\|_\infty \lesssim N^{(k,k,d+1)}(a; r, l) \,,$$

with an implicit constant only depending on d, r and l_0.

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

Corollary 2.11 [33, Corollary 4.7](case $d = 1$). *For any two open bounded intervals K, J as well as numbers $q \in (0,1]$ and $\alpha \geq 2$, the following estimate holds*

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

with a constant independent of α.

The next proposition gives an estimate for terms of the form $\chi_\Lambda \mathrm{Op}_\alpha(a)(1 - \chi_\Lambda)$, which we will come up when applying Lemmata 2.6 or 2.8. In order to state it, we first need to introduce the following condition.

Condition 2.12 [25, Condition 3.1]. *For $d \geq 1$, the set $\Lambda \subset \mathbb{R}^d$, satisfies one of the following requirements:*

- *(1) If $d = 1$, then Λ is a finite union of open intervals (bounded or unbounded) such that their closures are pair-wise disjoint.*
- *(2) If $d \geq 2$, then Λ is a Lipschitz region (i.e., an open set whose boundary is locally Lipschitz), and either Λ or $\mathbb{R}^d \setminus \Lambda$ is bounded.*

Proposition 2.13 [25, Proposition 3.2](Adapted to the cases needed and our notation). *Let the region $\Lambda \subset \mathbb{R}^d$ satisfy Condition 2.12, and let $\alpha_0 > 0$ be a constant. Let $q \in (0,1]$ and*

$$\tilde{m} := \lceil (d+1)q^{-1} \rceil + 1 \,.$$

Let a be a scalar-valued symbol only depending on $\boldsymbol{\xi}$, i.e., $a(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\xi}) \equiv a(\boldsymbol{\xi})$ with support contained in $B_\tau(\boldsymbol{\mu})$ for some $\boldsymbol{\mu} \in \mathbb{R}^d$ and $\tau > 0$. Assume that $a \in S^{(\tilde{m})}(\mathbb{R}^d)$ and $\mathrm{Op}_\alpha(a)$ is well defined with integral representation extending to all Schwartz functions. Then, for any $\alpha\tau \geq \alpha_0$,

$$\|\chi_\Lambda \mathrm{Op}_\alpha(a)(1 - \chi_\Lambda)\|_q \lesssim (\alpha\tau)^{\frac{d-1}{q}} N^{(\tilde{m})}(a; \tau) \,,$$

with implicit constants independent of a, α, τ and $\boldsymbol{\mu}$.

Proposition 2.14 [32, Proposition 3.8 and p. 17] with reference to [4, Theorem 11.1], [3, Section 5.8] and [31, Theorem 4.5]. *For $\boldsymbol{z} \in \mathbb{Z}$ set $\mathcal{C}_{\boldsymbol{z}} := \boldsymbol{z} + (0,1]^d$ and for $\sigma \in (0, \infty)$ and $g \in L^2_{\mathrm{loc}}(\mathbb{R}^d)$*

$$|g|_\sigma := \left[\sum_{\boldsymbol{z} \in \mathbb{Z}} \left(\int_{\mathcal{C}_{\boldsymbol{z}}} |g(x)|^2 \mathrm{d}x \right)^{\sigma/2} \right]^{1/\sigma} .$$

Then, given functions $a, h \in L^2_{\mathrm{loc}}(\mathbb{R})$ with $|a|_\sigma, |h|_\sigma < \infty$ for some $\sigma \in (0, 2)$, it follows that $h \, \mathrm{Op}_\alpha(a) \in \mathfrak{S}_\sigma$ (with integral representation extending to all Schwartz functions) and

$$\left\| h \, \mathrm{Op}_1(a) \right\|_\sigma \leq C \, |h|_\sigma \, |a|_\sigma \,.$$

3. The Regularized Projection Operator

3.1. Definition and Basic Properties

As previously mentioned, the entropy is computed using the mode-wise regularized projection operator to the negative frequency space $(\Pi_-^\varepsilon)_{kn}$. This operator emerges from $e^{-itH_{kn}}$ from Sect. 2.3.2 by setting $t = i\varepsilon$ (the "$i\varepsilon$"-regularization) and restricting to the negative frequencies. Similar as explained in Sect. 2.3.3, for operators of this form it suffices to consider the corresponding operator for one angular mode $(\Pi_-^\varepsilon)_{kn}$. So more precisely, for any $X \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$ the operator $(\Pi_-^\varepsilon)_{kn}$ is defined by

$$\left((\Pi_-^\varepsilon)_{kn} X\right)(x) := \frac{1}{\pi} \int_{-\infty}^0 d\omega\, e^{\varepsilon\omega} \sum_{a,b=1}^2 t_{ab}^{kn\omega} X_a^{kn\omega}(x) \langle X_b^{kn\omega} | X \rangle\,, \qquad (3.1)$$

for any $x \in \mathbb{R}$.

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

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

The asymptotics of the radial solutions at the horizon (Lemma 2.3) yield the following boundedness properties for the functions X_a^ω:

Remark 3.1. Given $u_2 \in \mathbb{R}$ and a constant $C > 0$, we consider measurable functions $X, Z : \mathbb{R} \to \mathbb{C}^2$ with the properties

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

Then the estimate in Lemma 2.3 yields

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

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

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. ◇

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:

Lemma 3.2. *Let N be a manifold with integration measure μ. Given a function $f \in L_{\mathrm{loc}}^1(N, \mathbb{C}^n)$ (with $n \in \mathbb{N}$), we assume that the corresponding functional on the test functions*

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

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

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

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

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

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

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

Lemma 3.3. *Equation (3.1) defines a continuous endomorphism $(\Pi_-^\varepsilon)_{kn}$ on L^2 $(\mathbb{R},\mathbb{C}^2)$ with operator norm*

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

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

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

Applying Remark 3.1, we may interchange integrations such that

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

Moreover, from [8, proof of Theorem 3.6] we obtain the estimate

$$\int_{-\infty}^\infty \frac{d\omega}{\pi} \left| \sum_{a,b=1}^2 t_{ab}^\omega \left\langle X \,\big|\, X_a^\omega\right\rangle\left\langle X_b^\omega \,\big|\, Z\right\rangle \right| \leq \|X\|\|Z\| , \qquad (3.2)$$

which yields

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

Now by Lemma 3.2 we conclude that

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

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

3.2. Functional Calculus for H_{kn}

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

$$(\Pi^\varepsilon_-)_{kn} = g(H_{kn}),$$

for some suitable function g.

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

Proposition 3.4. *Let $g \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$ be a 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*

$$\big(g(H_{kn})X\big)(u) = \int_{-\infty}^\infty \frac{d\omega}{\pi}\, g(\omega) \int_{-\infty}^\infty du' \sum_{a,b=1}^2 t_{ab}^\omega\, X_a(u,\omega)\, \langle X_b(u',\omega)$$
$$\times \big|\, X(u')\big\rangle_{\mathbb{C}^2}, \tag{3.3}$$

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

$$\langle Z \,|\, g(H)X \rangle = \int_{-\infty}^\infty \frac{d\omega}{\pi}\, g(\omega) \sum_{a,b=1}^2 t_{ab}^\omega\, \langle Z|X_a^\omega\rangle\langle X_b^\omega|X\rangle, \tag{3.4}$$

Proposition 3.5. *Let $g \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$ be a real valued function. Then the operator $g(H_{kn})$ has the following properties:*

(i) *The operator norm of $g(H_{kn})$ is bounded, namely*

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

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

Proof of Proposition 3.4. We proceed in two steps.
First step: Proof for $g \in C_0^\infty(\mathbb{R})$: Since the Fourier transform is a bijection 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

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

We evaluate the right hand side of (3.3) 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 3.1. We thus obtain

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

Using the rapid decay of $\hat{g}$ together with (3.2), we can make use of the Fubini–Tonelli theorem which leads to

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

It is shown in [8] that

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

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 (3.2)), leading to

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

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 $\big(\sigma(H_{kn}), \Sigma, \mu\big)$. 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 $x \in A$ it holds that

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

which leads to

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

Thus, we conclude that for any $X, Z \in C_0^\infty(\mathbb{R} \times S^2, \mathbb{C}^4)$,

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

Then, Lemma 3.2 (together with similar estimates as before) yields that

$$\int_{-\infty}^{\infty} g(\omega) \sum_{a,b=1}^{2} t_{ab}^\omega X_a^\omega(.) \, \langle X_b^\omega | X \rangle \in L^2(\mathbb{R} \times S^2, \mathbb{C}^4) \, ,$$

and therefore

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

almost everywhere.

Second step: Proof for g $\in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$:   We choose 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 that[1]

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

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

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

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

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

So the function $\big(C + \|g\|_\infty\big) |U^{-1}X| \in L^2(A, \mu)$ dominates the sequence of measurable functions $\big(\mathcal{M}_{\Delta g_n \circ f}(U^{-1}X) \big)_{n\in\mathbb{N}}$ which additionally tends to zero pointwise almost everywhere. Therefore, using Lebesgue's dominated convergence theorem, we conclude that

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

and thus

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

In particular, we conclude that for any $X, Z \in C_0^\infty(\mathbb{R}, \mathbb{C}^4)$,

$$\langle Z \mid g_n(H_{kn})X \rangle \to \langle Z \mid g(H_{kn})X \rangle . \tag{3.5}$$

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

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

Now keep in mind that Remark 3.1 also yields the bound

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

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

---

[1] Note 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 $\|g\|_\infty + 1$ (to ensure uniform boundedness) and then going over to a subsequence (to get pointwise convergence a.e., see, for example, [30, Theorem 3.12]).

$$|(**)| \leq \int_{-\infty}^{\infty} d\omega \big|\Delta g_n(\omega)\big| \Big| \sum_{a,b=1}^{2} t_{ab}^{\omega} \langle Z | X_a^{kn\omega}\rangle \langle X_b^{kn\omega} | X\rangle \Big|$$

$$\leq C_{Z,X} \int_{-\infty}^{\infty} d\omega \big|\Delta g_n(\omega)\big| \overset{n\to\infty}{\longrightarrow} 0 \,.$$

Combined with (3.5), this finally yields for any $X, Z \in C_0^{\infty}(\mathbb{R} \times S^2, \mathbb{C}^4)$

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

We obtain (3.3) just as in the first case using Lemma 3.2. Finally, (3.4) follows by testing with Z and again interchanging the integrals as explained before. $\square$

Proof of Proposition 3.5. (i) This follows directly from (3.4) together with (3.2), since

$$|\langle Z \mid g(H_{kn})X\rangle_{L^2}| \overset{(3.4)}{=} \Big| \int \frac{d\omega}{\pi}\, g(\omega) \sum_{a,b=1}^{2} t_{ab}^{\omega} \langle Z \mid X_a^{\omega}\rangle_{L^2} \langle X_b^{\omega} \mid X\rangle_{L^2} \Big| \quad (3.6)$$

$$\overset{(3.2)}{\leq} \|g\|_{\infty} \|Z\|_{L^2} \|X\|_{L^2} \,. \tag{3.7}$$

(ii) Using (3.3), the following computation shows that the operator $g(H_{kn})$ is also self-adjoint because for any $X, Z \in \Xi$ we have

$$\langle Z \mid g(H_{kn})X\rangle_{L^2}$$

$$= \int du \int \frac{d\omega}{\pi}\, g(\omega) \int du' \sum_{a,b=1}^{2} \overline{t_{ba}^{\omega}\, \langle X(u') \mid X_b(u',\omega)\rangle_{\mathbb{C}^2}} \langle X_a(u,\omega) \mid Z(u)\rangle_{\mathbb{C}^2}$$

$$\overset{\text{Fubini}}{=} \overline{\int du' \int \frac{d\omega}{\pi}\, g(\omega) \int du \sum_{a,b=1}^{2} t_{ba}^{\omega}\, \langle Z(u) \mid X_b(u,\omega)\rangle_{\mathbb{C}^2} \langle X_a(u',\omega) \mid X(u')\rangle_{\mathbb{C}^2}}$$

$$= \overline{\langle X \mid g(H_{kn})Z\rangle_{L^2}} = \langle g(H_{kn})Z \mid X\rangle_{L^2} \,.$$

Note that applying Fubini is justified in view of Remark 3.1. From this equation, the self-adjointness follows by continuous extension. $\square$

Now we apply these results to the operator Π_-^{ε}:

Corollary 3.6. *Consider the function*

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

then we have

$$(\Pi_-^{\varepsilon})_{kn} = g(H_{kn})$$

Moreover, for η_κ as before we have:

$$\eta_\kappa((\Pi_-^{\varepsilon})_{kn}) = (\eta_\kappa \circ g)(H_{kn}) \tag{3.8}$$

Proof. First of all note that

$$(\Pi^\varepsilon_-)_{kn} = g(H_{kn}) \,,$$

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 3.4) and are bounded (see Lemma 3.3 and Proposition 3.5). Equation (3.8) then follows by applying the functional calculus of H_{kn} (which is applicable due to Proposition 3.5). $\qquad\square$

3.3. Representation as a Pseudo-Differential Operator

The general idea is to rewrite Π^ε_- in the form of $\mathrm{Op}_\alpha(\mathcal{A})$ and identify α with the inverse regularization constant:

$$\alpha = \frac{l_0}{\varepsilon} \,,$$

with a suitable reference length l_0.

With the help of (3.3), we obtain for any $\psi \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$

$$\big((\Pi^\varepsilon_-)_{kn}\psi\big)(u) = \int_{-\infty}^\infty (\Pi^\varepsilon_-)_{kn}(u, u') \, \psi(u') \, \mathrm{d}u'$$

with the kernel

$$(\Pi^\varepsilon_-)_{kn}(u, u') = \frac{1}{\pi} \int_{-\infty}^\infty e^{-i\omega(u-u')} \left[\begin{pmatrix} \mathfrak{a}_{\varepsilon,11}(\omega) & \mathfrak{a}_{\varepsilon,12}(u, \omega) \\ \mathfrak{a}_{\varepsilon,21}(u, \omega) & \mathfrak{a}_{\varepsilon,22}(\omega) \end{pmatrix} + \mathcal{R}_0(u, u', \omega) \right]$$
$$\mathrm{d}\omega \tag{3.9}$$

and

$$\mathfrak{a}_{\varepsilon,11}(\omega) = e^{\varepsilon\omega} \left(\big|f_{0,1}^+(\omega)\big|^2 \chi_{(-m,0)}(\omega) + \frac{1}{2} \chi_{(-\infty,-m)}(\omega) \right)$$

$$\mathfrak{a}_{\varepsilon,12}(u, \omega) = e^{-\varepsilon\omega} e^{2i\omega u} \left(\overline{f_{0,1}^-(-\omega)} \, f_{0,1}^+(-\omega) \, \chi_{(0,m)}(\omega) + t_{12}(-\omega) \, \chi_{(m,\infty)}(\omega) \right)$$

$$\mathfrak{a}_{\varepsilon,21}(u, \omega) = e^{\varepsilon\omega} e^{2i\omega u} \left(f_{0,1}^-(\omega) \, \overline{f_{0,1}^+(\omega)} \, \chi_{(-m,0)}(\omega) + t_{21}(\omega) \, \chi_{(-\infty,-m)}(\omega) \right)$$

$$\mathfrak{a}_{\varepsilon,22}(\omega) = e^{-\varepsilon\omega} \left(\big|f_{0,1}^-(\omega)\big|^2 \chi_{(0,m)}(\omega) + \frac{1}{2} \chi_{(m,\infty)}(\omega) \right) \,,$$

and some error term $\mathcal{R}_0(u, u', \omega)$ related to the error term $R_0(u)$ in Lemma 2.3. A more detailed computation is given in Appendix C. Moreover, the more precise form of $\mathcal{R}_0(u, u', \omega)$ is found in Sect. 6.1.3. Note that for the Schwarzschild case we always replace $\boldsymbol{x}$ by u and $\boldsymbol{y}$ by u' to emphasize that we are working with Regge–Wheeler coordinates.

In order to bring $(\Pi^\varepsilon_-)_{kn}$ in the form of $\mathrm{Op}_\alpha(\mathcal{A})$, we need to rescale the ω-integral by a dimensionless parameter α. As previously mentioned, the idea is to set $\alpha = l_0/\varepsilon$ with some reference length l_0. In Schwarzschild space, the only scaling parameter of the geometry is the mass of the black hole M. Thus, we choose as reference length $l_0 = M$ and rescale the ω integral by

$$\alpha := \frac{M}{\varepsilon} \,.$$

Introducing the notation

$$\xi := \frac{\omega}{\alpha} = \frac{\varepsilon \omega}{M} ,$$

we thereby obtain

$$
(\Pi_-^\varepsilon)_{kn}(u, u') = \frac{\alpha}{\pi} \int e^{-i\alpha\xi(u-u')} \left[\begin{pmatrix} \mathfrak{a}_{\varepsilon,11}(M\xi/\varepsilon) & \mathfrak{a}_{\varepsilon,12}(u, M\xi/\varepsilon) \\ \mathfrak{a}_{\varepsilon,21}(u, M\xi/\varepsilon) & \mathfrak{a}_{\varepsilon,22}(M\xi/\varepsilon) \end{pmatrix} \right.
$$
$$
\left. + \mathcal{R}_0(u, u', (M\xi/\varepsilon)) \right] d\xi ,
\tag{3.10}
$$

and set

$$\mathcal{R}_0^{(\varepsilon)}(u, u', \xi) := \mathcal{R}_0(u, u', (M\xi/\varepsilon)) \tag{3.11}$$

$$\mathcal{A}^{(\varepsilon)}(u, \xi) := \begin{pmatrix} \mathfrak{a}_{\varepsilon,11}(M\xi/\varepsilon) & \mathfrak{a}_{\varepsilon,12}(u, M\xi/\varepsilon) \\ \mathfrak{a}_{\varepsilon,21}(u, M\xi/\varepsilon) & \mathfrak{a}_{\varepsilon,22}(M\xi/\varepsilon) \end{pmatrix} . \tag{3.12}$$

Note that in the matrix-valued functions a_ε and $\mathcal{R}_0$ we use the scaling parameter ε and otherwise α. This is convenient because we will first consider the $\alpha \to \infty$ limit of an operator related to the $\varepsilon \to 0$ limit of $\mathcal{A}^{(\varepsilon)}$ and then estimate the errors caused by this procedure. In this sense, α and ε can at first be considered independent scaling parameters. When considering the limiting case $\varepsilon \to 0$ however, one has to keep their relation in mind.

4. The Regularized Fermionic Vacuum State and Its Entanglement Entropy

After the above preparations, we can now define the regularized fermionic vacuum state in the Schwarzschild geometry as well as the corresponding (Rényi) entanglement entropy of the event horizon. Our starting point is the observation that a quasi-free fermionic state is uniquely described by its reduced one-particle density operator D (see Definition 2.1). We want to choose D as the regularized projection operator onto all the negative-frequency solutions of the Dirac equation. Using the spectral calculus for the Hamiltonian H in the Dirac equation in the Hamiltonian form (2.10), our first ansatz is

$$D = g(H) \qquad \text{with} \qquad g(\omega) := \chi_{(-\infty,0)}(\omega) \, e^{\varepsilon\omega} . \tag{4.1}$$

Note that, in the limiting case $\varepsilon \searrow 0$, the operator D goes over to the projection operator to all negative-frequency solutions. The corresponding quasi-free state Ω is pure. In the case $\varepsilon > 0$, the function $e^{\varepsilon\omega}$ gives a smooth cutoff for large frequencies on the energy scale $1/\varepsilon$. Even in this regularized situation, the spectral function g is discontinuous at $\omega = 0$. This implements the physical picture that, in the vacuum, all negative frequency one-particle states are occupied, whereas all positive frequency states are not.

Our fist ansatz (4.1) has the shortcoming that it involves an infinite number of angular momentum modes, giving rise to a divergence in (1.9). In order to remedy the situation, we let $\mathcal{O}$ be a finite subset of $(\mathbb{Z} + 1/2) \times \mathbb{N}$

(referred to as the *occupied angular momentum modes* or *occupied one-particle states*) and choose

$$D = \Pi_-^\varepsilon := \sum_{(k,n) \text{ occupied}} (\Pi_-^\varepsilon)_{kn} \,, \tag{4.2}$$

where we sum over all $(k,n) \in \mathcal{O}$. Here the mode-wise regularized projection operator $(\Pi_-^\varepsilon)_{kn}$ is defined using the integral representation by (3.1). Alternatively and equivalently, it can be characterized using the spectral calculus as described in Corollary 3.6.

We note that, for simplicity, for each angular momentum mode we choose the same regularization length ε. More generally, one could consider a regularized vacuum state where $\varepsilon = \varepsilon(k,n)$ depends on the angular mode. Since the entropy can be decomposed into the sum of the entropies of all angular momentum modes, all our results generalize immediately to this more general state.

Choosing D according to (4.2), we consider the (Rényi) entanglement entropy as defined by (2.2), where Λ is chosen as an annular region in (1.4); see also Fig. 2. Note that in the Regge–Wheeler coordinates the horizon is located at $-\infty$, so ultimately we want to consider the limit $u_0 \to -\infty$ and $\rho \to \infty$.

As explained in Sect. 2.3.3, we can compute the trace mode-wise by going over to the subregions $\mathcal{K}$:

$$\text{tr} \left(\eta_\kappa \big(\chi_\Lambda \Pi_-^\varepsilon \big) \chi_\Lambda \big) - \chi_\Lambda \eta_\kappa \big(\Pi_-^\varepsilon \big) \chi_\Lambda \right) = \sum_{\substack{(k,n) \\ \text{occupied}}} \text{tr} \left(\eta_\kappa \big(\chi_\mathcal{K} (\Pi_-^\varepsilon)_{kn} \chi_\mathcal{K} \big) \right.$$
$$\left. - \chi_\mathcal{K} \eta_\kappa \big((\Pi_-^\varepsilon)_{kn} \big) \chi_\mathcal{K} \big) \right).$$

Thus, we define the mode-wise Rényi entropy of the black hole as in (1.6) by

$$S_{\kappa,kn}^{\text{BH}} = \frac{1}{2} \lim_{\rho \to \infty} \lim_{\alpha \to \infty} \frac{1}{\tilde{f}(\alpha)} \lim_{u_0 \to -\infty} \text{tr}\, \Delta_\kappa \big((\Pi_-^\varepsilon)_{kn}, \mathcal{K} \big) \,,$$

where $\tilde{f}(\alpha)$ is a function describing the highest order of divergence in α (we will later see that here $\tilde{f}(\alpha) = \log \alpha$). The complete entanglement entropy of the black hole is then the sum over all occupied modes (see (1.9)).

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

$$\lim_{\rho \to \infty} \lim_{\alpha \to \infty} \frac{1}{f(\alpha)} \lim_{u_0 \to -\infty} \text{tr} \left(\eta_\kappa \big(\chi_\mathcal{K} (\Pi_-^\varepsilon)_{kn} \chi_\mathcal{K} \big) - \chi_\mathcal{K} \eta_\kappa \big((\Pi_-^\varepsilon)_{kn} \big) \chi_\mathcal{K} \right) \tag{4.3}$$

$$= \lim_{\rho \to \infty} \lim_{\alpha \to \infty} \frac{1}{f(\alpha)} \lim_{u_0 \to -\infty} \text{tr} \left(\eta_\kappa \big(\chi_\mathcal{K} \text{Op}_\alpha(\mathcal{A}_0) \chi_\mathcal{K} \big) - \chi_\mathcal{K} \eta_\kappa \big(\text{Op}_\alpha(\mathcal{A}_0) \big) \chi_\mathcal{K} \right), \tag{4.4}$$

where

$$\mathcal{A}_0(\xi) := \begin{pmatrix} e^{M\xi} \chi_{(-\infty,0)}(\xi) & 0 \\ 0 & e^{-M\xi} \chi_{(0,\infty)}(\xi) \end{pmatrix}. \tag{4.5}$$

(We will later see that the operators in (4.3) and (4.4) are well defined and trace class). The notation $\mathcal{A}_0$ is supposed to emphasize the connection to the $\varepsilon \to 0$
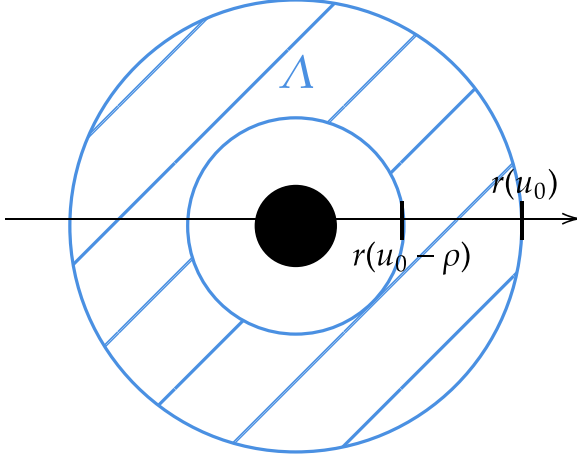
FIGURE 2. Cross section visualizing the set $\Lambda = \mathcal{K} \times S^2$

limit of A_ε. Since $\mathcal{A}_0$ is diagonal, the computation of (4.4) is much easier than the one for (4.3). In fact, we have

$$(4.4) = \sum_{j=1}^{2} \lim_{\rho \to \infty} \lim_{\alpha \to \infty} \frac{1}{f(\alpha)} \lim_{u_0 \to -\infty} \mathrm{tr} \left(\eta_\kappa \big(\chi_\mathcal{K} \mathrm{Op}_\alpha(\mathfrak{a}_{0,j}) \chi_\mathcal{K} \big) - \chi_\mathcal{K} \eta_\kappa \big(\mathrm{Op}_\alpha(\mathfrak{a}_{0,j}) \big) \chi_\mathcal{K} \right)$$

with the scalar functions

$$\mathfrak{a}_{0,1}(\xi) := e^{M\xi} \chi_{(-\infty,0)}(\xi) \qquad \text{and} \quad \mathfrak{a}_{0,2}(\xi) := e^{-M\xi} \chi_{(0,\infty)}(\xi) \,. \tag{4.6}$$

This reduces the computation of (4.4) to a problem for real-valued symbols for which many results are already established.

Remark 4.1. We point out that our definition of the entanglement entropy differs from the conventions in [20,24] in that we do not add the entropic difference operator of the complement of Λ. This is justified as follows. On the technical level, our procedure is easier, because it suffices to consider compact spatial regions (indeed, we expect that the entropic difference operator on the complement of Λ is not trace class). Conceptually, restricting attention to the entropic difference operator of Λ 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 the entropic difference operator (1.3).

This qualitative argument can be made more precise with the following formal computation, which shows that at least the unregularized entropic difference is the same for the inner and the outer parts: First of all note that $\eta_\kappa(x)$ vanishes at $x = 0$ and $x = 1$. Since Π_- is a projection, this means that

$$\eta_\kappa(\Pi_-) = 0 \qquad \text{and therefore} \qquad \mathrm{tr} \left(\chi_\Lambda \, \eta_\kappa(\Pi_-) \, \chi_\Lambda \right)$$
$$= 0 = \mathrm{tr} \left(\chi_{\Lambda^c} \, \eta_\kappa(\Pi_-) \, \chi_{\Lambda^c} \right).$$

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

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

which yields

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

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

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

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 $\eta_\kappa(\Pi_-\,\chi_\Lambda\,\Pi_-)$ and $\eta_\kappa(\chi_\Lambda\,\Pi_-\,\chi_\Lambda)$, proving that

$$\mathrm{tr}\,\eta_\kappa(\chi_\Lambda\,\Pi_-\,\chi_\Lambda) = \mathrm{tr}\,\eta_\kappa(\Pi_-\,\chi_\Lambda\,\Pi_-)\,.$$

Due to the symmetry of η_κ, namely

$$\eta_\kappa(x) = \eta_\kappa(1-x) \qquad\text{for any } x\in\mathbb{R}\,,$$

this then leads to

$$\begin{aligned}
\mathrm{tr}\,\eta_\kappa(\chi_\Lambda\,\Pi_-\,\chi_\Lambda) &= \mathrm{tr}\,\eta_\kappa(\Pi_-\,\chi_\Lambda\,\Pi_-) = \mathrm{tr}\,\eta_\kappa\big(\Pi_- - \Pi_-\,\chi_\Lambda\,\Pi_-\big)\\
&= \mathrm{tr}\,\eta_\kappa(\Pi_-\,\chi_{\Lambda^c}\,\Pi_-)\,.
\end{aligned}$$

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

$$\mathrm{tr}\,\eta_\kappa(\chi_\Lambda\,\Pi_-\,\chi_\Lambda) = \mathrm{tr}\,\eta_\kappa(\Pi_-\,\chi_{\Lambda^c}\,\Pi_-) = \mathrm{tr}\,\eta_\kappa(\chi_{\Lambda^c}\,\Pi_-\,\chi_{\Lambda^c})\,.$$

Regularizing this expression suggests that the entanglement entropies of the inside and outside as defined in (1.3) coincide. If this is the case, our definition of entanglement entropy agrees (up to a numerical factor) with that in [20, 24]. ◇

5. Trace of the Limiting Operator

In this section, we shall analyze the operator $\mathrm{Op}_\alpha(\mathfrak{a}_{0,1})$ in (4.6). Of course, the same methods apply to $\mathrm{Op}_\alpha(\mathfrak{a}_{0,2})$.

Notation 5.1. In the following, it might happen that in the symbol $\mathcal{A}$ we can factor out a characteristic function in ξ, i.e.,

$$\mathcal{A}(u, u', \xi) = \chi_\Omega(\xi)\,\tilde{\mathcal{A}}(u, u', \xi)\,.$$

In this case, we will sometimes denote the characteristic function in ξ corresponding to the set Ω by I_Ω (this is to avoid confusion with the characteristic function $\chi_\mathcal{K}$ in the variables u or u').
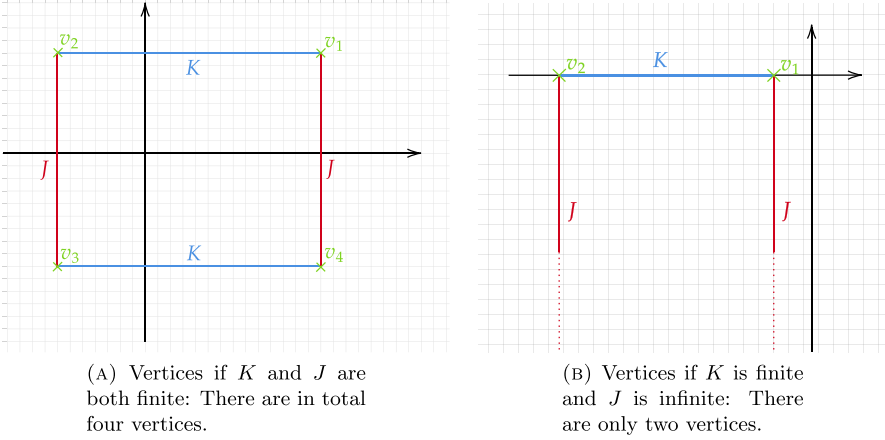
(A) Vertices if K and J are both finite: There are in total four vertices.

(B) Vertices if K is finite and J is infinite: There are only two vertices.

FIGURE 3. Illustration with examples of the "vertices" in Theorem 5.3

Remark 5.2. Note that the operator $\mathrm{Op}_\alpha(\mathfrak{a}_{0,1})$ corresponds to

$$\mathrm{Op}_\alpha(\mathfrak{a}_{0,1}) = \mathcal{F}\,\mathfrak{a}_{0,1}\,\mathcal{F}^{-1}\,,$$

and is therefore well defined on all of $L^2(\mathbb{R})$ and by Remark A.2 its integral representation extends to all Schwartz functions. Moreover, for any bounded subset $U \subseteq \mathbb{R}$ the integral representation of the operator $\chi_U \mathrm{Op}_\alpha(\mathfrak{a}_{0,1})\chi_U$ holds on all of $L^2(\mathbb{R})$ due to Lemma A.6. ◇

5.1. Idea for Smooth Functions

The general idea is to make use of the following one-dimensional result by Widom [39].

Theorem 5.3. *Let $K, J \subseteq \mathbb{R}$ intervals, $f \in C^\infty(\mathbb{R})$ be 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*

$$A(b) := \frac{1}{2}\Big(\chi_K\,\mathrm{Op}_\alpha\big(I_J\,b\big)\,\chi_K + \big(\chi_K\mathrm{Op}_\alpha\big(I_J\,b\big)\chi_K\big)^*\Big)\,, \qquad (5.1)$$

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

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

where v_i are the vertices of $K \times J$ (see Fig. 3)
    and

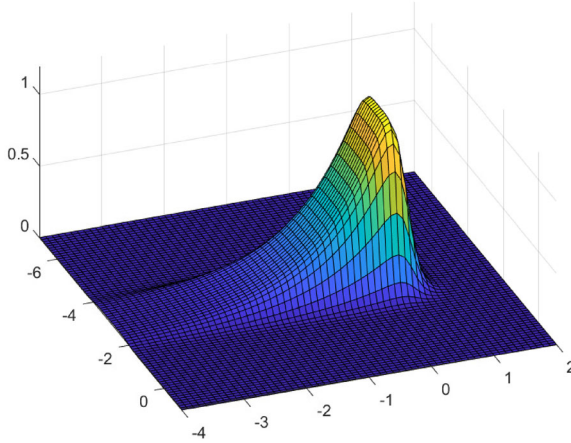$$U(c; f) := \int_0^1 \frac{1}{t(1-t)}\Big(f(tc) - tf(c)\Big)\,\mathrm{d}t \qquad \text{for any } c \in \mathbb{R}\,.$$

FIGURE 4. Plot of the function a in (5.3)

Remark 5.4. (i) To be precise, Widom considered operators with kernels

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

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

(ii) Moreover, Widom considers operators of the form $\mathrm{Op}_\alpha(a)$ whose integral representation extends to all of $L^2(K)$. We note that, in view of Lemma A.6, this assumption holds for any operator $\mathrm{Op}_\alpha(a)$ with Schwartz symbol $a = a(x,\xi)$, even if, apriori, the integral representation holds only when inserting smooth compactly supported functions. $\diamond$

We want to apply the above theorem with $J = (-\infty, 0) =: \mathcal{J}$ and $K = \mathcal{K} = (u_0 - \rho, u_0)$, where we choose f as a suitable approximation of the function η_κ (again with $f(0) = 0$) and a as an approximation of the diagonal matrix entries $\mathfrak{a}_{0,1/2}$ in (4.5) and (4.6). For ease of notation, we only consider $a \approx \mathfrak{a}_{0,1}$, noting that our methods apply similarly to $\mathfrak{a}_{0,2}$. To be more precise, we first introduce the smooth non-negative cutoff functions $\Psi, \Phi \in C^\infty(\mathbb{R})$ with

$$\Psi(\xi) = \begin{cases} 1, & \xi \leq 0 \\ 0, & \xi > 1 \end{cases} \qquad \text{and} \qquad \Phi(u) = \begin{cases} 1, & u \in [-\rho, 0] \\ 0, & u \notin (-\rho - 1, 1) \end{cases}, \tag{5.2}$$

and set $\Phi_{u_0}(x) := \Phi(x - u_0)$. Then we may introduce a as the function

$$\mathfrak{a}(u,\xi) := \Psi(\xi) \, \Phi_{u_0}(u) \, e^{M\xi} . \tag{5.3}$$

For a plot of a see Fig. 4.

Note that then $\mathfrak{a}$ is a Schwartz function and

$$\chi_K \, \mathrm{Op}_\alpha(I_J \, \mathfrak{a}) \, \chi_K = \chi_K \, \mathrm{Op}_\alpha(\mathfrak{a}_{0,1}) \, \chi_K . \tag{5.4}$$

Moreover, the resulting symbol clearly fulfills the condition of Lemma A.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 A.1. This implies that we can leave out the symmetrization in (5.1), i.e.,

$$A(\mathfrak{a}) = \chi_K \operatorname{Op}_\alpha(I_J \, \mathfrak{a}) \, \chi_K = \chi_K \operatorname{Op}_\alpha(\mathfrak{a}_{0,1}) \, \chi_K \,. \tag{5.5}$$

Furthermore, due to Lemma A.1, we may pull out any function f as in Theorem 5.3 in the sense that

$$\chi_K \operatorname{Op}_\alpha(I_J \, f(\mathfrak{a})) \, \chi_K = \chi_K \operatorname{Op}_\alpha(f(\mathfrak{a}_{0,1})) \, \chi_K = \chi_K \, f(\operatorname{Op}_\alpha(\mathfrak{a}_{0,1})) \, \chi_K \,,$$

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

In our application, the vertices of $K \times J$ are (similar as in Fig. 3B) given by

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

and thus

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

leading to

$$\operatorname{tr}\left(f\big(\chi_K \operatorname{Op}_\alpha(\mathfrak{a}_{0,1}) \chi_K\big) - \chi_K f\big(\operatorname{Op}_\alpha(\mathfrak{a}_{0,1})\big) \chi_K \right) = \frac{1}{2\pi^2} \, \log(\alpha) \, U(1; f) + \mathcal{O}(1) \,, \tag{5.6}$$

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

Note that, using Lemma A.3 and the fact that $\mathfrak{a}_{0,1}$ 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 $u_0 \to -\infty$. We need to keep this in mind because we shall take the limit $u_0 \to -\infty$ before the limit $\alpha \to \infty$ (cf. (1.6)).

5.2. Proof for Non-differentiable Functions

In order to state the main result of this section, we first need to introduce the following condition.

Condition 5.5. *Let $T := \{t_0, \ldots, t_l\}$ be a finite set and $g \in C^2(\mathbb{R} \setminus T) \cap C^0(\mathbb{R})$ 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*

$$|g^{(t)}(x)| \le c_k \, |t - t_i|^{\gamma - k} \,. \tag{5.7}$$

Example 5.6. As shown in detail in Lemma D.1, the functions η_κ satisfy Condition 5.5 with $T = \{0, 1\}$ and if $\kappa \ne 1$ for any $\gamma \le \min\{1, \kappa\}$ if $\kappa = 1$ we may take any $\gamma < 1$. ◇

The following theorem constitutes the main result of this section.

Theorem 5.7. *Let $\mathcal{K} = (u_0 - \rho, u_0)$, $\mathcal{J} = (-\infty, 0)$ (as in Sect. 5.1) and $\mathfrak{a}_{0,1}(\xi) = e^{M\xi} \chi_{(-\infty, 0)}(\xi)$ as in (4.6). Moreover, let $g \in C^2(\mathbb{R} \setminus \{t_0, \ldots, t_l\}) \cap C^0(\mathbb{R})$ satisfy Condition 5.5 with $g(0) = 0$. Then*

$$\lim_{\alpha \to \infty} \lim_{u_0 \to -\infty} \frac{1}{\log \alpha} \operatorname{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) = \frac{1}{2\pi^2} \, U(1; g) \,. \tag{5.8}$$

In the proof of Theorem 5.7, we will apply Lemmata 2.6 and 2.8. In order to complete the error estimates, one finally needs to control the term $\|PA(\mathbb{1} - P)|^\sigma\|_{\mathfrak{S}}$. This can be done with the following lemma.

Lemma 5.8. *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 $\mathfrak{a}_{0,1}$ from (4.6) satisfies*

$$\left\| \chi_\mathcal{K} \operatorname{Op}_\alpha(\mathfrak{a}_{0,1}) (1 - \chi_\mathcal{K}) \right\|_q^q \lesssim \log \alpha .$$

with implicit constants independent of α and u_0.

Proof. First of all, make use Lemma A.3 in order to replace the region $\mathcal{K}$ by $\mathcal{K}_0 := (-\rho, 0)$:

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

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 $\operatorname{supp} \Psi_0 \subseteq (-\frac{1}{2}, \frac{3}{2})$. For any $j \in \mathbb{Z}$, we consider the symbols

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

Using the notation $\mathcal{J}_j := (j-1, j)$ for any $j \in \mathbb{Z}_{\leq 0}$, we obtain with the help of Lemma A.8 together with Remark A.9,

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

so with the triangle inequality (2.15) we conclude that

$$\left\| \chi_{\mathcal{K}_0} \operatorname{Op}_\alpha(\mathfrak{a}_{0,1}) (1 - \chi_{\mathcal{K}_0}) \right\|_q^q \leq \sum_{j \in \mathbb{Z}_{\leq 0}} \left\| \chi_{\mathcal{K}_0} P_{\mathcal{J}_j, \alpha} \operatorname{Op}_\alpha(\mathfrak{a}_j) (1 - \chi_{\mathcal{K}_0}) \right\|_q^q . \quad (5.9)$$

In the next step, we want to interchange $P_{\mathcal{J}_j, \alpha}$ and $\chi_{\mathcal{K}_0}$. To this end note that

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

where we also used that

$$\left(\chi_{\mathcal{K}_0} P_{\mathcal{J}_j, \alpha} (1 - \chi_{\mathcal{K}_0}) \right)^* = (1 - \chi_{\mathcal{K}_0}) P_{\mathcal{J}_j, \alpha} \chi_{\mathcal{K}_0} ,$$

together with the fact that singular values (and therefore the q-norm) are invariant under Hermitian conjugation.[2] Moreover, using Remark A.4 together with Corollary 2.11 we conclude that for any $j \in \mathbb{Z}_{\leq 0}$:

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

---

[2] Note that for any $A \in \mathfrak{S}_q$ we can write $\|A\|_q = (\sum_i \sqrt{\lambda_i}^q)^{1/q}$ where the λ_i are the eigenvalues of $A^* A$ (note that since A is compact, there are countably many). Moreover, for any eigenvector ψ of $A^* A$ corresponding to a non-zero eigenvalue, the vector $A\psi$ is an eigenvector of AA^* with the same eigenvalue, so we see that $\|A^*\|_q \leq \|A\|_q$ (as ψ might lie in the kernel of A). Then, symmetry yields the equality.

with implicit constant independent of $j \in \mathbb{Z}_{\leq 0}$, $\alpha \geq 2$ and u_0. Moreover, making use of Lemma 2.10 together with Remark A.2 and the fact that

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

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

$$\|\mathrm{Op}_\alpha(\mathfrak{a}_j)\|_\infty^q \lesssim e^{qMj} ,$$

again with an implicit constant independent of j and α. Using the Hölder-type inequality (2.16), this allows us to estimate

$$\begin{aligned}
\|\chi_{\mathcal{K}_0} \, P_{\mathcal{J}_j,\alpha} \, \mathrm{Op}_\alpha(\mathfrak{a}_j) \, (1 - \chi_{\mathcal{K}_0})\|_q^q &\leq \|[\chi_{\mathcal{K}_0}, \, P_{\mathcal{J}_j,\alpha}] \, \mathrm{Op}_\alpha(\mathfrak{a}_j) \, (1 - \chi_{\mathcal{K}_0})\|_q^q \\
&+ \|P_{\mathcal{J}_j,\alpha} \, \chi_{\mathcal{K}_0} \, \mathrm{Op}_\alpha(\mathfrak{a}_j) \, (1 - \chi_{\mathcal{K}_0})\|_q^q \leq \|[\chi_{\mathcal{K}_0}, \, P_{\mathcal{J}_j,\alpha}]\|_q^q \|\mathrm{Op}_\alpha(\mathfrak{a}_j) \, (1 - \chi_{\mathcal{K}_0})\|_\infty^q \\
&+ \|P_{\mathcal{J}_j,\alpha}\|_\infty^q \|\chi_{\mathcal{K}_0} \, \mathrm{Op}_\alpha(\mathfrak{a}_j) \, (1 - \chi_{\mathcal{K}_0})\|_q^q \lesssim e^{qMj} \log \alpha \\
&+ \|\chi_{\mathcal{K}_0} \, \mathrm{Op}_\alpha(\mathfrak{a}_j) \, (1 - \chi_{\mathcal{K}_0})\|_q^q .
\end{aligned}$$

with an implicit constant independent of $j \in \mathbb{N}_0$ and $\alpha \geq 2$. Thus, it remains to estimate the term $\|\chi_{\mathcal{K}_0} \, \mathrm{Op}_\alpha(\mathfrak{a}_j) \, (1 - \chi_{\mathcal{K}_0})\|_q^q$. To this end, we want to apply Proposition 2.13 to $\mathfrak{a}_j$. So choose $\tau = 2$ and $\boldsymbol{\mu} = j - 1/2$, then

$$N^{(\tilde{m})}(\mathfrak{a}_j; \tau) \lesssim e^{Mj} ,$$

with an implicit constant independent of j. This yields

$$\begin{aligned}
\|\chi_{\mathcal{K}_0} \, P_{\mathcal{J}_j,\alpha} \, \mathrm{Op}_\alpha(\mathfrak{a}_j) \, (1 - \chi_{\mathcal{K}_0})\|_q^q &\leq \|[\chi_{\mathcal{K}_0}, \, P_{\mathcal{J}_j,\alpha}] \, \mathrm{Op}_\alpha(\mathfrak{a}_j) \, (1 - \chi_{\mathcal{K}_0})\|_q^q \\
&\lesssim e^{qMj} \log \alpha ,
\end{aligned}$$

(5.10)

with an implicit constant independent of j and $\alpha \geq 3$. Then, summarizing (5.9) and (5.10) yields

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

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

In the proof of Theorem 5.7, we will also make use of the following continuity result for $U(1; f)$.

Lemma 5.9. *Let f be a function on $[0,1]$ with $f(0) = 0$.*

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

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

Then,

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

(ii) *If f satisfies Condition 5.5 with $X = \{z\}$ where $z = 0$ or $z = 1$ and is supported in $[z - R, z + R]$ 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:

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

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

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

and therefore

$$(\mathrm{I}) \leq \int_0^{1/2} \underbrace{\left| \frac{1}{(1 - t)} \right|}_{\leq 2} \left(\underbrace{|f'(0)|}_{\leq \|f\|_{C^2}} + \underbrace{|t/2|}_{\leq 1/4} \underbrace{|f''(\tilde{t})|}_{\leq \|f\|_{C^2}} \right) \mathrm{d}t + \int_0^{1/2} \underbrace{\left| \frac{1}{(1 - t)} \right|}_{\leq 2} \underbrace{|f(1)|}_{\leq \|f\|_{C^2}} \mathrm{d}t$$

$$\leq \frac{9}{4} \|f\|_{C^2}$$

(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 $t = 1$,

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

We thus obtain

$$(\mathrm{II}) \leq \int_{1/2}^1 \left| \frac{1}{t(1 - t)} \right| \left(|1 - t| \, |f(1)| + |1 - t| \, |f'(1)| + \frac{|1 - t|^2}{2} |f''(\tilde{t})| \right) \mathrm{d}t$$

$$\leq \int_{1/2}^1 \underbrace{|1/t|}_{\leq 2} \left(\underbrace{|f(1)|}_{\leq \|f\|_{C^2}} + \underbrace{|f'(1)|}_{\leq \|f\|_{C^2}} + \underbrace{\frac{|1 - t|}{2}}_{\leq 1/4} \underbrace{|f''(\tilde{t})|}_{\leq \|f\|_{C^2}} \right) \mathrm{d}t \leq \frac{9}{4} \|f\|_{C^2} .$$

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

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

This yields for $R < 1/2$,

$$|(\mathrm{I})| = \left| \int_0^{1/2} \frac{1}{t(1 - t)} f(t) \mathrm{d}t \right| \leq \int_0^R \underbrace{\frac{1}{|1 - t|}}_{\leq 1/(1 - R)} \|f\|_2 |t|^{\gamma - 1} \mathrm{d}t$$

$$\leq \frac{1}{1-R} \|f\|_2 \underbrace{\int_0^R |t|^{\gamma-1} \, \mathrm{d}t}_{=R^\gamma/\gamma} \leq \|f\|_2 \frac{R^\gamma}{\gamma(1-R)} \,,$$

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

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

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

Moreover, just as in the previous case, one can estimate

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

This yields for $R < 1/2$,

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

$\square$

Now we have all the tools to prove Theorem 5.7.

Proof of Theorem 5.7. Before beginning, we note that the u_0-limit in (5.8) may be disregarded, because the symbol is translation invariant in position space (see Lemma A.3, noting that $\mathfrak{a}_{0,1}$ does not depend on $u \equiv \boldsymbol{x}$ or $u' \equiv \boldsymbol{y}$).

The remainder of the proof is based on the idea of the proof of [34, Theorem 4.4] Let $\mathfrak{a}$ be the symbol in (5.3). By Lemma 2.10, we can assume that the operator norm of $\mathrm{Op}_\alpha(\mathfrak{a})$ is uniformly bounded in α. We want to apply Lemma A.8 with $\mathcal{A} = \mathfrak{a}$ 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 A.9 (i) yields condition (ii), whereas condition (i) follows from the estimate

$$\int \mathrm{d}u \left| \int \mathrm{d}\xi \, e^{-i\xi u} \, e^{M\xi} \, \psi(\xi) \, \Psi(\xi) \, \Phi_{u_0}(u) \right|^2$$
$$\leq \int_{u_0-\rho-1}^{u_0+1} \mathrm{d}u \left(\int \mathrm{d}\xi \, \chi_{(-\infty,1)}(\xi) \, e^{M\xi} \, |\psi(\xi)| \right)^2$$
$$\leq (\rho+2) \, \|\chi_{(-\infty,1)} \, e^{\cdot/M}\|_{L^2(\mathbb{R},\mathbb{C})}^2 \, \|\psi\|_{L^2(\mathbb{R},\mathbb{C})}^2 \,,$$

(which holds for any $\psi \in L^2(\mathbb{R})$). Now Lemma A.8 yields

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

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

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

uniformly in α (recall that $A(\mathfrak{a})$ is the symmetric localization from Theorem 5.3). Moreover, the sup-norm of the symbol $\mathfrak{a}_{0,1}$ 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

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

possibly replacing g by the function

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

with a smooth cutoff function $\Psi_C \geq 0$ such that $\Psi_C|_{[-C+1, C-1]} \equiv 1$ and $\operatorname{supp} \Psi_C \subseteq [-C, C]$. For ease of notation, we will write $g \equiv \tilde{g}$ in what follows.

We remark that the function η_κ which we plan to consider later already satisfies this property by definition with $C = 2$. From Lemma 2.8 and Lemma 5.8 we see that $D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1})$ is indeed trace class. We now compute this trace, proceeding in two steps.

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

To this end, we first apply the Weierstrass approximation theorem as given in [27, Theorem 1.6.2] to obtain a polynomial g_δ such that $f_\delta := g - g_\delta$ fulfills

$$\max_{0 \leq k \leq 2} \max_{|t| \leq C} \big| f_\delta^{(k)}(t) \big| \leq \delta \,. \tag{5.11}$$

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 Lemma 2.6 with $n = 2$, $r = C$, some $\sigma \in (0, 1)$, $q = 1$ and

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

(note that here g is the function in Lemma 2.6) where Ψ_C is the cutoff function from before (the cutoffs and approximation are visualized in Fig. 5).

This gives

$$\big\| f_\delta\big(\chi_\mathcal{K} \operatorname{Op}_\alpha(\mathfrak{a}_{0,1}) \, \chi_\mathcal{K}\big) - \chi_\mathcal{K} \, f_\delta\big(\operatorname{Op}_\alpha(\mathfrak{a}_{0,1})\big) \, \chi_\mathcal{K} \big\|_1$$
$$= \big\| \tilde{f}_\delta\big(\chi_\mathcal{K} \operatorname{Op}_\alpha(\mathfrak{a}_{0,1}) \, \chi_\mathcal{K}\big) - \chi_\mathcal{K} \, \tilde{f}_\delta\big(\operatorname{Op}_\alpha(\mathfrak{a}_{0,1})\big) \, \chi_\mathcal{K} \big\|_1$$
$$\lesssim \delta \, \big\| \chi_\mathcal{K} \operatorname{Op}_\alpha(\mathfrak{a}_{0,1}) \, (1 - \chi_\mathcal{K}) \big\|_\sigma^\sigma \,.$$

with an implicit constant independent of δ and α. Moreover, applying Lemma 5.8 with $q = \sigma$, we conclude that for α large enough

$$\big\| f_\delta\big(\chi_\mathcal{K} \operatorname{Op}_\alpha(\mathfrak{a}_{0,1}) \, \chi_\mathcal{K}\big) - \chi_\mathcal{K} \, f_\delta(\operatorname{Op}_\alpha(\mathfrak{a}_{0,1})) \, \chi_\mathcal{K} \big\|_1 \lesssim \delta \, \log \alpha \,,$$

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

$$\operatorname{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) \leq \operatorname{tr} D_\alpha(g_\delta, \mathcal{K}, \mathfrak{a}_{0,1}) + \| D_\alpha(f_\delta, \mathcal{K}, \mathfrak{a}_{0,1}) \|_1$$
$$\leq \operatorname{tr} D_\alpha(g_\delta, \mathcal{K}, \mathfrak{a}_{0,1}) + C_3 \, \delta \, \log \alpha \,,$$

with a constant C_3 independent of δ and α. In order to compute the remaining trace, we can again apply Theorem 5.3 (exactly as in the example (5.6)). This gives

$$\operatorname{tr} D_\alpha(g_\delta, \mathcal{K}, \mathfrak{a}_{0,1}) = \frac{1}{2\pi^2} \log(\alpha) \, U(1; g_\delta) + \mathcal{O}(1) \,,$$
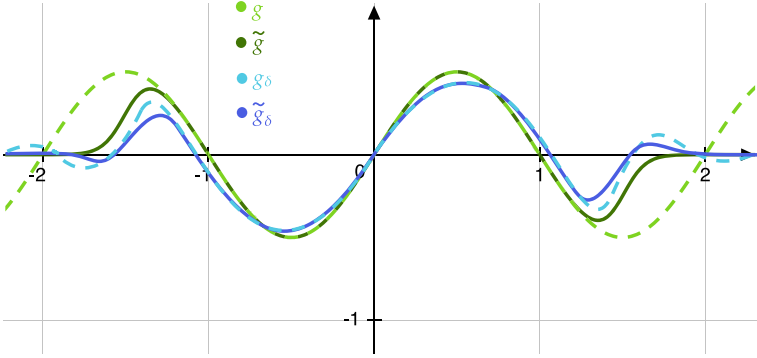
FIGURE 5. Visualization of the cutoffs and approximations in the first step of the proof of Theorem 5.7 for $C = 2$. We start with a function g, which is first multiplied by the cutoff-function Ψ_C, giving $\tilde{g}$. This function is then approximated by a polynomial g_δ. Multiplying g_δ by the cutoff function Ψ_C results in a function which is here called $\tilde{g}_\delta$ (but does not directly appear in the proof). The function $\tilde{f}_\delta$ is then given by the difference between $\tilde{g}$ and $\tilde{g}_\delta$

and thus

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

which yields together with Lemma 5.9,

$$\limsup_{\alpha \to \infty} \frac{1}{\log \alpha} \operatorname{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) \leq \frac{1}{2\pi^2} U(1; g_\delta) + C_3 \, \delta \,. \qquad (5.12)$$

Moreover, applying Lemma 5.9 to f_δ we obtain due the (5.11)

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

Therefore, taking the limit $\delta \to 0$ in (5.12) gives

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

Analogously, using

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

we obtain

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

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

$$\liminf_{\alpha \to \infty} \frac{1}{\log \alpha} \operatorname{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) \geq \frac{1}{2\pi^2} U(1; g) \,.$$
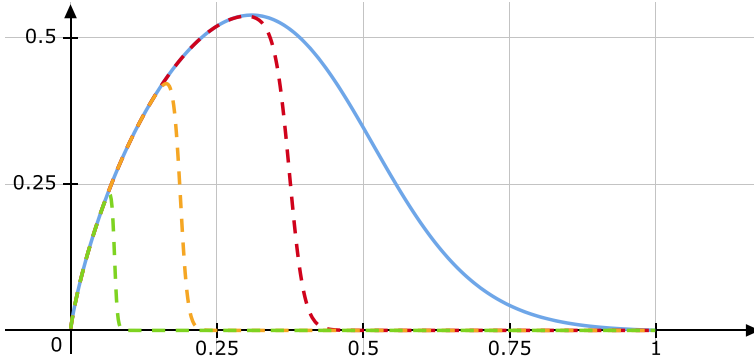
FIGURE 6. Schematic plot of a function g (blue) which is non-differentiable at $z = 0$ with the corresponding functions $g_{1/2}^{(1)}$ (red), $g_{1/4}^{(1)}$ (orange) and $g_{1/10}^{(1)}$ (green): They are cutting out the non-differentiable point

Combining the inequalities for the $\limsup$ and $\liminf$, we conclude that for any $g \in C^2(\mathbb{R})$,

$$\lim_{\alpha \to \infty} \frac{1}{\log \alpha} \operatorname{tr} D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) = \frac{1}{2\pi^2} U(1; g) . \tag{5.13}$$

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 $\xi \in C_0^\infty(\mathbb{R})$ 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

$$g_R^{(1)}(t) := g(t)\, \xi\big((t - z)/R\big) \quad \Rightarrow \quad \operatorname{supp} g_R^{(1)} \subseteq [z - R, z + R] ,$$
$$g_R^{(2)}(t) := g(t) - g_R^{(1)}(t) \quad \Rightarrow \quad \operatorname{supp} g_R^{(2)} \subseteq [-C, C] ;$$

see also Fig. 6.

Note that the derivatives of $g_R^{(1)}$ satisfy the bounds

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

(with some numerical constants $c(n,k)$) and therefore the norm $\lfloor . \rfloor_2$ in Lemma 2.8 can be estimated by

$$\lfloor g_R^{(1)} \rfloor_2 = \max_{0 \leq k \leq 2} \sup_{t \neq z} \left| \sum_{n=0}^{k} c(n,k)\, g^{(k-n)}(t)\, \xi^{(n)}\big((t-z)/R\big)\, \frac{1}{R^n} \right| \cdot |t-z|^{-\gamma+k}$$

$$\leq \max_{0 \leq k \leq 2} \sup_{t \neq z} \sum_{n=0}^{k} |c(n,k)|\, \big|g^{(k-n)}(t)\big|\, |t-z|^{-\gamma+k-n}\, \big|\xi^{(n)}\big((t-z)/R\big)\big|$$

$$\frac{|t-z|^n}{R^n}\,.$$

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

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

we conclude that

$$\lfloor g_R^{(1)} \rfloor_2 \leq C_4 \lfloor g \rfloor_2 \tag{5.14}$$

with C_4 independent of R (also note that $\lfloor g \rfloor_2$ 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 (5.13) to the function $g_R^{(2)}$ (which clearly is in $C^2(\mathbb{R})$),

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

Next, we apply Lemma 2.8 to $g_R^{(1)}$ with A and P as before and some $\sigma \in (0,1)$ with $\sigma < \gamma$,

$$\big\| D_\alpha\big(g_R(1), \mathcal{K}, \mathfrak{a}_{0,1}\big) \big\|_1 \leq C_\sigma \lfloor g \rfloor_2\, R^{\gamma-\sigma}\, \big\| \chi_\mathcal{K}\, \mathrm{Op}_\alpha(\mathfrak{a}_{0,1})\,(1-\chi_\mathcal{K}) \big\|_\sigma^\sigma\,.$$

Applying Lemma 5.8 (for α large enough) with $q = \sigma$ yields

$$\big\| D_\alpha\big(g_R(1), \mathcal{K}, \mathfrak{a}_{0,1}\big) \big\|_1 \leq C_5\, \lfloor g \rfloor_2\, R^{\gamma-\sigma}\, \log \alpha\,.$$

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

$$\limsup_{\alpha \to \infty} \frac{1}{\log \alpha}\, \mathrm{tr}\, D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) \leq U\big(1; g_R^{(2)}\big) + C_5\, \lfloor g \rfloor_2\, R^{\gamma-\sigma}$$

$$\liminf_{\alpha \to \infty} \frac{1}{\log \alpha}\, \mathrm{tr}\, D_\alpha(g, \mathcal{K}, \mathfrak{a}_{0,1}) \geq U\big(1; g_R^{(2)}\big) + C_5\, \lfloor g \rfloor_2\, R^{\gamma-\sigma}\,.$$

The end result follows just as before by taking the limit $R \to 0$, provided that we can show the convergence $U(1; g_R^{(2)}) \to U(1; g)$ for $R \to 0$. 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 $\lim_{R \to 0} U(1; g - g_R^{(2)}) = 0$ 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 5.9, which also yields due to (5.14),

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

This concludes the proof. □

We finally apply Theorem 5.7 to the function η_κ and the matrix-valued symbol $\mathcal{A}_0$ (see (1.2) and (4.5)).

Corollary 5.10. *For any $\kappa > 0$, η_κ, $\mathcal{K}$ and $\mathcal{A}_0$ as before,*

$$\lim_{\alpha \to \infty} \lim_{u_0 \to \infty} \frac{1}{\log \alpha} \operatorname{tr} D_\alpha(\eta_\kappa, \mathcal{K}, \mathcal{A}_0) = \frac{1}{\pi^2} U(1; \eta_\kappa) = \frac{1}{6} \frac{\varkappa + 1}{\varkappa} \,.$$

Moreover, in the case that $\kappa = 1$, we can explicitly compute the coefficient $U(1; \eta_1)$ to give

$$\lim_{\alpha \to \infty} \lim_{u_0 \to \infty} \frac{1}{\log \alpha} \operatorname{tr} D_\alpha(\eta_1, \mathcal{K}, \mathcal{A}_0) = \frac{1}{\pi^2} U(1; \eta_1) = \frac{1}{3} \,.$$

Proof. As explained in Example 5.6, the functions η_κ satisfy Condition 5.5 with $n = 2$ for any $\kappa > 0$. Moreover, we have $\eta_\kappa(0) = 0$ for any $\kappa > 0$. Therefore, we can apply Theorem 5.7 and obtain

$$\lim_{\alpha \to \infty} \lim_{u_0 \to \infty} \frac{1}{\log \alpha} \operatorname{tr} D_\alpha(\eta_\kappa, \mathcal{K}, \mathfrak{a}_{0,1}) = \frac{1}{2\pi^2} U(1; \eta_\kappa) \,.$$

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

$$\lim_{\alpha \to \infty} \lim_{u_0 \to \infty} \frac{1}{\log \alpha} \operatorname{tr} D_\alpha(\eta_\kappa, \mathcal{K}, \mathfrak{a}_{0,2}) = \frac{1}{2\pi^2} U(1; \eta_\kappa) \,,$$

and therefore

$$\lim_{\alpha \to \infty} \lim_{u_0 \to \infty} \frac{1}{\log \alpha} \operatorname{tr} D_\alpha(\eta_\kappa, \mathcal{K}, \mathcal{A}_0) = \frac{1}{\pi^2} U(1; \eta_\kappa) \,.$$

By [23, Appendix], evaluating $U(1; \eta_\kappa)$ yields

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

and therefore

$$\lim_{\varepsilon \searrow 0} \lim_{u_0 \to \infty} \frac{1}{\ln(1/\varepsilon)} \operatorname{tr} D_\alpha(\eta_\kappa, \mathcal{K}, \mathcal{A}_0) = \frac{1}{\pi^2} U(1; \eta_\kappa) = \frac{1}{6} \frac{\kappa + 1}{\kappa} \,.$$

This concludes the proof. □

Corollary 5.10 already looks quite similar to Theorem 1.1. The remaining task is to show equality in (4.4). To this end, we need to show that all the correction terms drop out in the limits $u_0 \to \infty$ and $\alpha \to \infty$. The next section is devoted to this task.

6. Estimating the Error Terms

In the previous section, we worked with the simplified kernel (4.5) and computed the corresponding entropy. In this section, we estimate all the errors, thereby proving the equality in (4.4). Our procedure is summarized as follows. Using (3.10), the regularized projection operator $(\Pi_-^\varepsilon)_{kn}$ can be written as

$$(\Pi_-^\varepsilon)_{kn} = \mathrm{Op}_\alpha\big(2\,(\mathcal{A}^{(\varepsilon)} + \mathcal{R}_0^{(\varepsilon)})\big)$$

and $\mathcal{A}^{(\varepsilon)}$ as in (3.12) and the error term

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

We denote the corresponding symbol by

$$\big((\mathfrak{a}_{\mathrm{full}})_{ij}\big)_{1 \le i,j \le 2} := \mathcal{A}_{\mathrm{full}}^{(\varepsilon)} := 2(\mathcal{A}^{(\varepsilon)} + \mathcal{R}_0^{(\varepsilon)})\,.$$

In preparation, translate $\mathcal{K}$ to $\mathcal{K}_0$ with the help of the unitary operator T_{u_0} making use of Lemma A.3. Moreover, we use that the operators $(\Pi_-^\varepsilon)_{kn}$ and $\mathrm{Op}_\alpha(\mathcal{A}_0)$ are self-adjoint. We thus obtain

$$D_\alpha(\eta_\kappa, \mathcal{K}, \mathcal{A}_{\mathrm{full}}^{(\varepsilon)}) - D_\alpha(\eta_\kappa, \mathcal{K}, \mathcal{A}_0) = D_\alpha(\eta_\kappa, \mathcal{K}_0, T_{u_0}(\mathcal{A}_{\mathrm{full}}^{(\varepsilon)}))$$
$$-D_\alpha(\eta_\kappa, \mathcal{K}_0, T_{u_0}(\mathcal{A}_0))\,,$$

where $\mathcal{A}_0$ is the kernel of the limiting operator from (4.5). Note that $T_{u_0}(\mathcal{A}_0) = \mathcal{A}_0$ since the symbol $\mathcal{A}_0$ only depends on ξ. Now we can estimate

$$\|D_\alpha(\eta_\kappa, \mathcal{K}_0, T_{u_0}(\mathcal{A}_{\mathrm{full}}^{(\varepsilon)})) - D_\alpha(\eta_\kappa, \mathcal{K}_0, \mathcal{A}_0)\|_1 \qquad\qquad\qquad \text{(I)}$$
$$\le \left\|\eta_\kappa\big(\chi_{\mathcal{K}_0}\,\mathrm{Op}_\alpha(T_{u_0}(\mathcal{A}_{\mathrm{full}}^{(\varepsilon)}))\,\chi_{\mathcal{K}_0}\big) - \eta_\kappa\big(\chi_{\mathcal{K}_0}\,\mathrm{Op}_\alpha(\mathcal{A}_0)\big)\,\chi_{\mathcal{K}_0}\big)\right\|_1$$

$$+ \left\|\chi_{\mathcal{K}_0}\,\big(\eta_\kappa\big(\mathrm{Op}_\alpha(T_{u_0}(\mathcal{A}_{\mathrm{full}}^{(\varepsilon)}))\big)\big) - \eta_\kappa\big(\mathrm{Op}_\alpha(\mathcal{A}_0)\big)\big)\,\chi_{\mathcal{K}_0}\right\|_1 . \qquad \text{(II)}$$

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

6.1. Estimate of the Error Term (I)

We begin with the following simplified result from [34], which is related to Lemma 2.8.

Theorem 6.1. *[34, Condition 2.3 and Theorem 2.4 (simplified to our needs)] Let f satisfy Condition 2.7 with some $n \ge 2$ and $\gamma, R > 0$. Let $\mathfrak{S}$ be a q-normed ideal of compact operators on $\mathfrak{H}$ such that there is $\sigma \in (0,1]$ with $\sigma < \gamma$ and*

$$(n - \sigma)^{-1} < q \le 1\,.$$

Let $\mathcal{A}, \mathcal{B}$ be two bounded self-adjoint operators on $\mathfrak{H}$. Suppose that $|\mathcal{A} - \mathcal{B}|^\sigma \in \mathfrak{S}$, then

$$\|f(\mathcal{A}) - f(\mathcal{B})\|_\mathfrak{S} \le C_n\,R^{\gamma - \sigma}\,\lfloor f \rfloor_n\,\big\||\mathcal{A} - \mathcal{B}|^\sigma\big\|_\mathfrak{S}$$

with a positive constant C_n independent of $\mathcal{A}, \mathcal{B}, f$ and R.

In order to apply this theorem to the functions η_κ, as in the proof of Theorem 5.7 we use a partition of unity. Similar as explained in Example 5.6, we need to choose $\gamma < 1$ for $\kappa = 1$ and $\gamma \leq \min\{1, \kappa\}$ otherwise. We will later see that with the methods in this work we can only estimate the error terms if $\kappa > 2/3$. 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 $\mathcal{A} = \chi_{\mathcal{K}_0} \mathrm{Op}_\alpha(T_{u_0}(\mathcal{A}_{\mathrm{full}}^{(\varepsilon)})) \chi_{\mathcal{K}_0}$ and $\mathcal{B} = \chi_{\mathcal{K}_0} \mathrm{Op}_\alpha(\mathcal{A}_0) \chi_{\mathcal{K}_0}$ (which are clearly bounded and self-adjoint), we obtain

$$\left\| \eta_\kappa \left(\chi_{\mathcal{K}_0} \mathrm{Op}_\alpha(T_{u_0}(\mathcal{A}_{\mathrm{full}}^{(\varepsilon)})) \chi_{\mathcal{K}_0} \right) - \eta_\kappa \left(\chi_{\mathcal{K}_0} \mathrm{Op}_\alpha(\mathcal{A}_0) \chi_{\mathcal{K}_0} \right) \right\|_1 \\ \leq C \left\| \chi_{\mathcal{K}_0} \mathrm{Op}_\alpha(T_{u_0}(\mathcal{A}_{\mathrm{full}}^{(\varepsilon)}) - \mathcal{A}_0) \chi_{\mathcal{K}_0} \right\|_\sigma^\sigma \tag{6.1}$$

with C independent of $\mathcal{A}$ and $\mathcal{B}$ (and thus in particular independent of u_0 and α).

For ease of notation, from now on we will denote

$$\left(\Delta(\mathfrak{a}_{ij})_{u_0}^{(\varepsilon)} \right)_{1 \leq i,j, \leq 2} := \Delta\mathcal{A}_{u_0}^{(\varepsilon)} := T_{u_0}(\mathcal{A}_{\mathrm{full}}^{(\varepsilon)}) - \mathcal{A}_0.$$

Note that the symbol of the $\mathrm{Op}_\alpha(.)$ in (6.1) is matrix valued. But, applying Remark 2.4 (ii), we obtain

$$\left\| \chi_{\mathcal{K}_0} \mathrm{Op}_\alpha(\Delta\mathcal{A}_{u_0}^{(\varepsilon)}) \chi_{\mathcal{K}_0} \right\|_\sigma^\sigma \leq \sum_{i,j=1}^{2} \left\| \chi_{\mathcal{K}_0} \mathrm{Op}_\alpha(\Delta(\mathfrak{a}_{ij})_{u_0}^{(\varepsilon)}) \chi_{\mathcal{K}_0} \right\|_\sigma^\sigma,$$

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

We now proceed by estimating the Schatten norms of the operators

$$\chi_{\mathcal{K}_0} \mathrm{Op}_\alpha(\Delta(\mathfrak{a}_{ij})_{u_0}^{(\varepsilon)}) \chi_{\mathcal{K}_0}.$$

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

$$(\Delta\mathfrak{a}_{11})_{u_0}^{(\varepsilon)}(u, u', \xi) = e^{M\xi} \chi_{(-m\varepsilon/M, 0)}(\xi) \left(2|f_{0,1}^+|^2 \left(\frac{M\xi}{\varepsilon} \right) - 1 \right) \\ + r_{11} \left(u + u_0, u' + u_0, \frac{M\xi}{\varepsilon} \right) \tag{6.2}$$

$$(\Delta\mathfrak{a}_{12})_{u_0}^{(\varepsilon)}(u, u', \xi) = 2e^{-M\xi} e^{2Mi\xi(u+u_0)/(\varepsilon)} \left[\overline{f_{0,1}^-} \left(\frac{-M\xi}{\varepsilon} \right) f_{0,1}^+ \left(\frac{-M\xi}{\varepsilon} \right) \chi_{(0, m\varepsilon/M)}(\xi) \right. \\ \left. + t_{12} \left(\frac{-M\xi}{\varepsilon} \right) \chi_{(m\varepsilon/M, \infty)}(\xi) \right] + r_{12} \left(u + u_0, u' + u_0, \frac{M\xi}{\varepsilon} \right) \tag{6.3}$$

$$(\Delta\mathfrak{a}_{21})_{u_0}^{(\varepsilon)}(u, u', \xi) = 2e^{M\xi} e^{2Mi\xi(u+u_0)/\varepsilon} \left[f_{0,1}^- \left(\frac{M\xi}{\varepsilon} \right) \overline{f_{0,1}^+} \left(\frac{M\xi}{\varepsilon} \right) \chi_{(-m\varepsilon/M, 0)}(\xi) \right. \\ \left. + t_{21} \left(\frac{M\xi}{\varepsilon} \right) \chi_{(-\infty, -m\varepsilon/M)}(\xi) \right] + r_{21} \left(u + u_0, u' + u_0, \frac{M\xi}{\varepsilon} \right) \tag{6.4}$$

$$(\Delta\mathfrak{a}_{22})_{u_0}^{(\varepsilon)}(u, u', \xi) = -e^{-M\xi}\chi_{(0,m\varepsilon/M)}(\xi)\Big(2|f_{0,1}^-|^2\Big(\frac{-M\xi}{\varepsilon}\Big) - 1\Big)$$
$$+ r_{22}\Big(u + u_0, u' + u_0, \frac{M\xi}{\varepsilon}\Big), \tag{6.5}$$

with $r_{ij}(u, u', \xi) = (\mathcal{R}_0(u, u', \xi))_{ij}$ 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 $u_0 \to -\infty$.

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 $u \leq u_0 \to -\infty$. And, finally, there are the r_{ij}-terms which decay rapidly in u and/or u'. Due to the triangle inequality (2.15), it will suffice to estimate each of these classes separately.

6.1.1. 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

$$e^{M\xi}\chi_{(-m\varepsilon/M,0)}(\xi)\Big(2|f_{0,1}^+|^2(M\xi/\varepsilon) - 1\Big) \qquad \text{in } \Delta(\mathfrak{a}_{11})_{u_0}^{(\varepsilon)}$$
$$-e^{-M\xi}\chi_{(0,m\varepsilon/M)}(\xi)\Big(2|f_{0,1}^-|^2(-M\xi/\varepsilon) - 1\Big) \quad \text{in } \Delta(\mathfrak{a}_{22})_{u_0}^{(\varepsilon)}.$$

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 2.14. As an example, consider

$$a^{(\varepsilon)}(\xi) := e^{M\xi}\chi_{(-m\varepsilon/M,0)}(\xi)\Big(2|f_{0,1}^+|^2(M\xi/\varepsilon) - 1\Big),$$

and

$$h := \chi_{\mathcal{K}},$$

which are both in $L_{\text{loc}}^2(\mathbb{R})$ because $|f_{0,1}^+|$ is bounded. Moreover, applying Lemma A.5 we obtain:

$$\big(\text{Op}_\alpha(a^{(\varepsilon)})\big)(u, u') = \big(\text{Op}_1(a_{(\varepsilon)})\big)(u, u'),$$

for

$$a_{(\varepsilon)}(\xi) := a^{(\varepsilon)}(\xi/\alpha) = e^{\varepsilon\xi}\,\chi_{(-m,0)}(\xi)\,\Big(2\big|f_{0,1}^+(\xi)\big|^2 - 1\Big),$$

which is again in $L_{\text{loc}}^2(\mathbb{R})$ for the same reasons as $a^{(\varepsilon)}$. Now we apply the Hölder-type inequality (2.16) and Proposition 2.14 with $p \in (0, 1)$ arbitrary to obtain

$$\big\|\chi_{\mathcal{K}_0}\text{Op}_\alpha(a^{(\varepsilon)})\,\chi_{\mathcal{K}_0}\big\|_p^p \leq \|\chi_{\mathcal{K}_0}\|_\infty^p\,\big\|\chi_{\mathcal{K}_0}\text{Op}_\alpha(a^{(\varepsilon)})\big\|_p^p$$
$$\leq \big\|\chi_{\mathcal{K}_0}\text{Op}_1(a_{(\varepsilon)})\big\|_p^p \leq C\,|\chi_{\mathcal{K}_0}|_p^p\,|a_{(\varepsilon)}|_p^p.$$

Next, noting that $\mathcal{K}_0 = (-\rho, 0) \subseteq (-\lceil\rho\rceil, 0)$, it follows that

$$|\chi_{\mathcal{K}_0}|_p^p \leq \sum_{-\lceil\rho\rceil}^{0} 1 = \lceil\rho\rceil \,.$$

Similarly, since $|a_{(\varepsilon)}(\omega)|$ is bounded by one,

$$|a_{(\varepsilon)}|_p^p \leq \sum_{-\lceil m\rceil}^{0} 1 \leq \lceil m\rceil \,.$$

Combining the last two inequalities, we conclude that

$$\|\chi_{\mathcal{K}_0} \, \mathrm{Op}_\alpha(a^{(\varepsilon)}) \, \chi_{\mathcal{K}_0}\|_p^p \leq C \lceil\rho\rceil \lceil m\rceil \,. \tag{6.6}$$

Completely similar for

$$\tilde{a}^{(\varepsilon)}(\xi) := -e^{-M\xi} \chi_{(0, m\varepsilon/M)}(\xi)$$

we obtain

$$\|\chi_{\mathcal{K}_0} \, \mathrm{Op}_\alpha(\tilde{a}^{(\varepsilon)}) \, \chi_{\mathcal{K}_0}\|_p^p \leq C \lceil\rho\rceil \lceil m\rceil \,, \tag{6.7}$$

for any $p \in (0,1)$ so in particular for $p = \sigma$. The estimates (6.6) and (6.7) show that the error terms with small support are bounded uniformly in u_0 and α. Therefore, dividing by $\log\alpha$ and taking the limit $\alpha \to \infty$, these error terms drop out.

6.1.2. Rapidly Oscillating Error Terms. After translating the symbol by u_0, these error terms are of the form

$$b^{(\varepsilon)}(u, \xi, \alpha) = e^{-M\xi} \, e^{2Mi\xi(u+u_0)/\varepsilon} \, g(M\xi/\varepsilon) \, \chi_{(0,\infty)}(\xi) \quad \text{or}$$
$$\tilde{b}^{(\varepsilon)}(u, \xi, \alpha) = e^{M\xi} \, e^{2Mi\xi(u+u_0)/\varepsilon} \, \tilde{g}(M\xi/\varepsilon) \, \chi_{(-\infty,0)}(\xi) \,,$$

for some functions $g, \tilde{g}$ which are measurable and bounded. They appear in $\Delta(\mathfrak{a}_{12})_{u_0}^{(\varepsilon)}$ and $\Delta(\mathfrak{a}_{21})_{u_0}^{(\varepsilon)}$. For simplicity, we restrict attention to the symbols of the form $b^{(\varepsilon)}$, but all estimates work the same for $\tilde{b}^{(\varepsilon)}$ in the same way. We will make use of the following results from [5, Theorem 4 on page 273 and p. 254, 263, 273], which adapted and applied to our case of interest can be stated as follows.

Theorem 6.2. *Let* $l \in \mathbb{N}_0$ *and* K *be an integral operator on* $L^2(\mathcal{K}_0)$ *(again with* $\mathcal{K}_0 = (-\rho, 0)$*) with kernel* k*, i.e., for any* $\psi \in L^2(\mathcal{K}_0)$*:*

$$(K\psi)(u) = \int_{\mathcal{K}_0} k(u, u') \, \psi(u') \, \mathrm{d}u' \,.$$

If $k(., u') \in W_2^l(\mathcal{K}_0)$ *for almost all* $u' \in \mathcal{K}_0$ *with*

$$\theta_2^2(t) := \int_{\mathcal{K}_0} \|k(., u')\|_{W_2^l(\mathcal{K}_0)}^2 \, \mathrm{d}u' < \infty \,,$$

then

$$K \in \mathfrak{S}_p \qquad \text{for } p > p' = (1/2 + l)^{-1}$$

and

$$\|K\|_p \leq C_{l,p}\, \theta_2(t)\,.$$

We want to apply this theorem for $p \in (0,1)$ arbitrary, thus let $l \in \mathbb{N}$ arbitrary. Moreover, in view of Lemma A.6, the integral representation corresponding to $\chi_{\mathcal{K}_0} \mathrm{Op}_\alpha(b^{(\varepsilon)}) \chi_{\mathcal{K}_0}$ may be extended to all of $L^2(\mathbb{R})$ and we may interchange the $\mathrm{d}\xi$ and $\mathrm{d}u'$ integrations. Thus, we need to estimate the norm θ_2 of the kernel of this operator. Thus, we consider kernels of the form

$$k_{u_0}^{(\varepsilon)}(u,u') := \frac{M}{2\pi\varepsilon} \int_0^\infty e^{iM\xi(u+u'+u_0)/\varepsilon}\, e^{-M\xi}\, g(M\xi/\varepsilon)\, \mathrm{d}\xi$$

$$= \frac{M}{2\pi} \int_0^\infty e^{iM\tilde{\xi}(u+u'+u_0)}\, e^{-\varepsilon M\tilde{\xi}}\, g(M\xi)\, \mathrm{d}\tilde{\xi}\,,$$

where we used the change of coordinates $\tilde{\xi} = \xi/\varepsilon$. Since g is bounded and the factor $e^{-\varepsilon M\tilde{\xi}}$ provides exponential decay, these kernels are always differentiable up to arbitrary orders with

$$\frac{\mathrm{d}^l}{\mathrm{d}u^l} k_{u_0}^{(\varepsilon)}(u,u') = \frac{1}{2\pi} \int_0^\infty (iM\tilde{\xi})^l\, e^{i\omega(u+u'+u_0)}\, e^{-\varepsilon\omega}\, g(\omega)\, \mathrm{d}\omega\,, \qquad \text{for any } l \in \mathbb{N}\,.$$

Our goal is to show that the limit $u_0 \to -\infty$ of $\theta_2\big(k_{u_0}^{(\varepsilon)}\big)$ is uniformly bounded in ε. To this end, we first note that

$$k_{u_0}^{(\varepsilon)}(u,u') = \mathcal{F}(h_{1,(\varepsilon)})(-u-u'-u_0)\,, \quad \frac{\mathrm{d}^l}{\mathrm{d}u^l} k_{u_0}^{(\varepsilon)}(u,u') = \mathcal{F}(h_{2,(\varepsilon)})(-u-u'-u_0)\,,$$

with

$$h_{1,(\varepsilon)}(\omega) := \frac{1}{2\pi}\, e^{-\varepsilon\omega}\, g(\omega)\, \chi_{(0,\infty)}(\omega)\,, \quad h_{l,(\varepsilon)}(\omega) := \frac{1}{2\pi}\, (i\omega)^l\, e^{-\varepsilon\omega}\, g(\omega)\, \chi_{(0,\infty)}(\omega)\,.$$

Now note that both $h_{1,(\varepsilon)}$ and $h_{l,(\varepsilon)}$ are in $L^1(\mathbb{R})$, so the Riemann–Lebesgue Lemma (see, for example, [6, Theorem 1]) tells us that for any $\delta > 0$ we can find $R = R(\varepsilon) > 0$ such that

$$\left|k_{u_0}^{(\varepsilon)}u,u')\right|, \left|\frac{\mathrm{d}^l}{\mathrm{d}u^l} k_{u_0}^{(\varepsilon)}(u,u')\right| \leq \delta \qquad \text{for } |u+u'+u_0| > R\,.$$

Keeping in mind that for $u_0 \leq 0$,

$$|u+u'+u_0| \geq |u_0| \qquad \text{for any } u, u' \in \mathcal{K}_0,$$

this is satisfied for $u_0 < -R(\varepsilon)$. This yields

$$\big\|k_{u_0}^{(\varepsilon)}(.,y)\big\|_{W_2^l(\mathcal{K}_0)}^2 \leq l\delta^2\rho\,,$$

which in turn leads to

$$\theta_2(k_{u_0}^{(\varepsilon)}) \leq \sqrt{l}\delta\rho\,,$$

and so

$$\lim_{u_0 \to \infty} \|\chi_{\mathcal{K}_0}\, \mathrm{Op}_\alpha(b^{(\varepsilon)})\, \chi_{\mathcal{K}_0}\|_p \leq C_{1,\sigma}\, \sqrt{l}\rho\delta\,,$$

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 $u_0 \to -\infty$.

We note for clarity that, since we take the limit $u_0 \to -\infty$ first, we do not need to worry about the dependence of the above estimate on ε.

6.1.3. 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 2.3 with an error term of the form

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

with

$$R_\pm(u) := f^\pm(u) - f_0^\pm$$

and $f^\pm$ as in (B.1). Using this asymptotics in the integral representation, the error terms in (6.2)–(6.5) can (similar as explained in Appendix C) computed to be

$$r_{11}(u, u', \omega) = \chi_{(-\infty,0)}(\omega)\, e^{\varepsilon\omega} \sum_{a,b=1}^{2} t_{ab}(\omega)$$
$$\times \left[f_{0,a}^+(\omega)\, \overline{R_{+,b}(u', \omega)} + R_{+,a}(u, \omega)\, \overline{f_{0,b}^+(\omega)} + R_{+,a}(u, \omega)\, \overline{R_{+,b}(u', \omega)} \right]$$

$$r_{12}(u, u', \omega) = \chi_{(0,\infty)}(\omega)\, e^{2i\omega u}\, e^{-\varepsilon\omega} \sum_{a,b=1}^{2} t_{ab}(-\omega) \times \left[f_{0,a}^+(-\omega)\, \overline{R_{-,b}(u', -\omega)} \right.$$
$$\left. + R_{+,a}(u, -\omega)\, \overline{f_{0,b}^-(-\omega)} + R_{+,a}(u, -\omega)\, \overline{R_{-,b}(u', -\omega)} \right]$$

$$r_{21}(u, u', \omega) = \chi_{(-\infty,0)}(\omega)\, e^{2i\omega u}\, e^{\varepsilon\omega} \sum_{a,b=1}^{2} t_{ab}(\omega)$$
$$\times \left[f_{0,a}^-(\omega)\, \overline{R_{+,b}(u', \omega)} + R_{-,a}(u, \omega)\, \overline{f_{0,b}^+(\omega)} + R_{-,a}(u, \omega)\, \overline{R_{+,b}(u', \omega)} \right]$$

$$r_{22}(u, u', \omega) = \chi_{(0,\infty)}(\omega)\, e^{-\varepsilon\omega} \sum_{a,b=1}^{2} t_{ab}(-\omega) \left[f_{0,a}^-(-\omega)\, \overline{R_{-,b}(u', -\omega)} \right.$$
$$\times \left. + R_{-,a}(u, -\omega)\, \overline{f_{0,b}^-(-\omega)} + R_{-,a}(u, -\omega)\, \overline{R_{-,b}(u', -\omega)} \right] .$$

In order to estimate these terms, the idea is to apply Theorem 6.2 (as well as the σ-triangle inequality) to each of these terms (with u and u' shifted by u_0) and then take the limit $u_0 \to -\infty$. 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 2.3 that for all $u < u_2$,

$$|R_\pm(u, \omega)| \le c e^{du} , \quad |\partial_u R_\pm(u, \omega)| \le cd e^{du} , \tag{6.8}$$

with constants $c, d > 0$ that can be chosen independently of ω (note that we always normalize the solutions by $|f_0| = 1$). Now for any $a, b \in \{1, 2\}$ we consider the symbol

$$c^{(\varepsilon)}(u, u', \xi) := \chi_{(-\infty,0)}(\xi)\, e^{M\xi}\, t_{ab}(M\xi/\varepsilon)\, f_{0,a}^+(M\xi/\varepsilon)\, \overline{R_{+,b}(u', M\xi/\varepsilon)}\, \chi_{\mathcal{K}}(u)\, \chi_{\mathcal{K}}(u') ,$$

which is contributing to $r_{11}(u, u', M\xi/\varepsilon)$ (note that we again rescaled here in order to get the correct prefactor $e^{-i\alpha\xi(u-u')}$). Translating by u_0 as before gives

$$\tilde{c}^{(\varepsilon)}(u, u', \xi) = c^{(\varepsilon)}(u + u_0, u' + u_0, \xi)$$
$$= \chi_{(-\infty,0)}(\xi)\, e^{M\xi}\, t_{ab}(M\xi/\varepsilon)\, f_{0,a}^+(M\xi/\varepsilon)$$
$$\overline{R_{+,b}(u' + u_0, M\xi/\varepsilon)}\, \chi_{\mathcal{K}_0}(u)\, \chi_{\mathcal{K}_0}(u')\,.$$

By Lemma A.6, the corresponding integral representation can be extended to all of $L^2(\mathbb{R})$, since R_+ is bounded uniformly in ω when restricted to the compact interval $\mathcal{K}_0$ due to Lemma 2.3, and the $e^{M\xi}$-factor provides exponential decay in ω. Moreover, Lemma A.6 again implies that we may interchange the $d\xi$ and du' integrations.

In order to estimate the corresponding error term, we apply Theorem 6.2 to the kernel

$$k_{u_0,\alpha}(u, u') := \frac{1}{2\pi} \int_{-\infty}^{0} e^{-i\omega(u-u')}\, e^{\varepsilon\omega}\, t_{ab}(\omega)\, f_{0,a}^+(\omega)\, \overline{R_{+,b}(u' + u_0, \omega)}\, d\omega$$

(note that we could leave out the $\chi_{\mathcal{K}_0}$-functions because in Theorem 6.2 we consider the operator on $L^2(\mathcal{K}_0)$; moreover, we rescaled back as before). This kernel is differentiable for similar reasons as before and

$$\frac{d}{du} k_{u_0,\alpha}(u, u') := \frac{1}{2\pi} \int_{-\infty}^{0} (-i\omega)\, e^{-i\omega(u-u')}\, e^{\varepsilon\omega}\, t_{ab}(\omega)\, f_{0,a}^+(\omega)\, \overline{R_{+,b}(u' + u_0, \omega)}\, d\omega\,.$$

Using again the estimates for $R_\pm$ in (6.8) yields for any $u, u' \in \mathcal{K}_0$:

$$|k_{u_0,\alpha}(u, u')| \leq \frac{ce^{d(u'+u_0)}}{2\pi} \int_{-\infty}^{0} e^{\varepsilon\omega}\, d\omega = \frac{ce^{d(u'+u_0)}}{2\pi\varepsilon}\,,$$

$$\left|\frac{d}{du} k_{u_0,\alpha}(u, u')\right| \leq \frac{ce^{d(u'+u_0)}}{2\pi} \int_{-\infty}^{0} |\omega|\, e^{\varepsilon\omega}\, d\omega = \frac{ce^{d(u'+u_0)}}{2\pi\varepsilon^2}\,,$$

where we used that $|t_{ab}|, |f_{0,1/2}^\pm| \leq 1$. Therefore,

$$\left\|k_{u_0,\alpha}(\cdot, u')\right\|_{W_2^1(\mathcal{K}_0)}^2 = \rho\left(\frac{c^2 e^{2d(u'+u_0)}}{4\pi^2\varepsilon^2} + \frac{c^2 e^{2d(u'+u_0)}}{4\pi^2\varepsilon^4}\right)$$

and thus

$$\theta_2^2(k) \leq \frac{\rho^2}{\varepsilon^2}\left(C_1 + C_2/\varepsilon^2\right) e^{2du_0}\,,$$

which makes clear that the corresponding error term vanishes in the limit $u_0 \to -\infty$.

We next consider a u-dependent contribution to r_{11} for some $a, b \in \{1, 2\}$ whose kernel of the form

$$k_2(u, u') := \frac{1}{2\pi} \int_{-\infty}^{0} e^{-i\omega(u-u')}\, e^{\varepsilon\omega}\, t_{ab}(\omega)\, R_{+,a}(u + u_0, \omega)\, \overline{f_{0,b}^+(\omega)}\, d\omega\,.$$

Differentiating with respect to u gives

$$\frac{\mathrm{d}}{\mathrm{d}u} k_2(u, u') := \frac{1}{2\pi} \int_{-\infty}^{0} e^{-i\omega(u-u')} \, e^{\varepsilon\omega} \, t_{ab}(\omega) \, \overline{f_{0,b}^+(\omega)}$$
$$\left(\partial_u R_{+,a}(u + u_0, \omega) - i\omega \, R_{+,a}(u + u_0, \omega) \right) \mathrm{d}\omega \,,$$

so that, similarly as before,

$$\left| k_2(u, u') \right| \leq \frac{c e^{d(u+u_0)}}{2\pi\varepsilon} \,,$$
$$\left| \frac{\mathrm{d}}{\mathrm{d}u} k_2(u, u') \right| \leq \left(\frac{c}{2\pi\varepsilon^2} + \frac{cd}{2\pi\varepsilon} \right) e^{d(u+u_0)} \,.$$

This gives

$$\left\| k_2(., u') \right\|_{W_2^1(\mathcal{K}_0)}^2 \leq \rho \, C(\varepsilon) \, e^{2du_0}$$

and thus

$$\theta_2(k_2)^2 \leq \rho^2 \, \tilde{C}(\varepsilon) \, e^{2du_0}$$

with a constant $C(\varepsilon)$ independent of u_0. This shows that the corresponding error term again vanishes as $u_0 \to \infty$.

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 $u_0 \to -\infty$.

6.2. Estimate of the Error Term (II)

It remains to estimate the error terms (II) on page 43. First of all note that due to Lemma A.3,

$$\left\| \chi_{\mathcal{K}_0} \left(\eta_\kappa \left(\mathrm{Op}_\alpha \left(T_{u_0}(\mathcal{A}_{\mathrm{full}}^{(\varepsilon)}) \right) \right) - \eta_\kappa (\mathrm{Op}_\alpha(\mathcal{A}_0)) \right) \chi_{\mathcal{K}_0} \right\|_1$$
$$= \left\| \chi_{\mathcal{K}} \left(\eta_\kappa \left((\Pi_-^\varepsilon)_{kn} \right) - \eta_\kappa (\mathrm{Op}_\alpha(\mathcal{A}_0)) \right) \chi_{\mathcal{K}} \right\|_1$$

Luckily, in this case we can directly compute $\eta_\kappa \left((\Pi_-^\varepsilon)_{kn} \right)$ and $\eta_\kappa \left(\mathrm{Op}_\alpha(\mathcal{A}_0) \right)$, which simplifies the estimate. As explained before in Lemma A.1, we have

$$\eta_\kappa \left(\mathrm{Op}_\alpha(\mathcal{A}_0) \right) = \mathrm{Op}_\alpha \left(\eta_\kappa(\mathcal{A}_0) \right).$$

Moreover, from Proposition 3.4 and Corollary 3.6 we conclude that for any $\psi \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$,

$$\left(\eta_\kappa \left((\Pi_-^\varepsilon)_{kn} \right) \psi \right)(u) = \frac{1}{\pi} \int_{-\infty}^{0} \eta_\kappa(e^{\varepsilon\omega}) \sum_{a,b=1}^{2} t_{ab}(\omega) \, X_a(u, \omega) \left\langle X_b(., \omega) \mid \psi \right\rangle \mathrm{d}\omega \,.$$

So we conclude that we can rewrite

$$\eta_\kappa \left(\mathrm{Op}_\alpha(a_0) \right) - \eta_\kappa \left((\Pi_-^\varepsilon)_{kn} \right) = \mathrm{Op}_\alpha(\Delta\tilde{\mathcal{A}}^{(\varepsilon)}) \,,$$

where the entries of the symbol $\tilde{\mathcal{A}}^{(\varepsilon)} = (\Delta\tilde{\mathfrak{a}}_{i,j}^{(\varepsilon)})_{1\leq i,j\leq 2}$ are given by

$$\Delta\tilde{\mathfrak{a}}_{1,1}^{(\varepsilon)}(u, u', \xi) = \eta_\kappa\left(e^{M\xi}\right) e^{-M\xi} \left(\Delta\mathfrak{a}_{11}\right)_0^{(\varepsilon)}(\xi) \,,$$

$$\Delta\tilde{\mathfrak{a}}_{1,2}^{(\varepsilon)}(u, u', \xi) = \eta_\kappa\left(e^{-M\xi}\right) e^{M\xi} \, \Delta\mathfrak{a}_{12})_0^{(\varepsilon)}(u, \xi) \,,$$

$$(\Delta\tilde{\mathfrak{a}}_{2,1}^{(\varepsilon)}(u, u', \xi) = \eta_\kappa\left(e^{M\xi}\right) e^{-M\xi} \left(\Delta\mathfrak{a}_{21}\right)_0^{(\varepsilon)}(\xi) \,,$$

$$\Delta\tilde{\mathfrak{a}}_{2,2}^{(\varepsilon)}(u, u', \xi) = \eta_\kappa\left(e^{-M\xi}\right) e^{M\xi} \left(\Delta\mathfrak{a}_{22}\right)_0^{(\varepsilon)}(u, \xi) \,.$$

Thus, these error terms are almost the same as before, except that the factor $e^{M\xi}$ has been replaced by $\eta_\kappa(e^{M\xi})$ etc. and without translation by u_0. Therefore, after applying Lemma A.3 in order to again translate by u_0,

$$\left\|\chi_{\mathcal{K}} \left(\eta_\kappa\left((\Pi_-^\varepsilon)_{kn}\right) - \eta_\kappa\left(\mathrm{Op}_\alpha(\mathcal{A}_0)\right)\right) \chi_{\mathcal{K}}\right\|_1 = \left\|\chi_{\mathcal{K}_0} \, \mathrm{Op}_\alpha\left(T_{u_0}(\tilde{\mathcal{A}}^{(\varepsilon)})\right) \chi_{\mathcal{K}_0}\right\|_1 \,,$$

we can use the same techniques as before if we can show that the functions

$$g_1(\omega) := \eta_\kappa\left(e^{-\varepsilon\omega}\right) \chi_{(0,\infty)}(\omega) \,, \qquad g_2(\omega) := \omega \, \eta_\kappa\left(e^{-\varepsilon\omega}\right) \chi_{(0,\infty)}(\omega) \,,$$

are bounded and in $L^1(\mathbb{R})$ (and the same for the functions with $\omega \to -\omega$, but for simplicity we again omit this case). We start with the case that $\kappa = 1$ and first rewrite these functions in more detail as

$$g_1(\omega) = \chi_{(0,\infty)}(\omega) \left(\varepsilon\omega \, e^{-\varepsilon\omega} + \left(e^{-\varepsilon\omega} - 1\right) \log\left(1 - e^{-\varepsilon\omega}\right)\right)$$

$$g_2(\omega) = \chi_{(0,\infty)}(\omega) \, \omega \left(\varepsilon\omega \, e^{-\varepsilon\omega} + \left(e^{-\varepsilon\omega} - 1\right) \log\left(1 - e^{-\varepsilon\omega}\right)\right) \,.$$

The terms $e^{-\varepsilon\omega}\omega^k$ with $k = 1, 2$ are clearly bounded and in $L^1(\mathbb{R})$. Moreover,

$$\lim_{\omega\searrow 0} \left(\left(e^{-\varepsilon\omega} - 1\right) \log\left(1 - e^{-\varepsilon\omega}\right)\right)$$

$$= \lim_{\omega\searrow 0} \frac{\log\left(1 - e^{-\varepsilon\omega}\right)}{\left(e^{-\varepsilon\omega} - 1\right)^{-1}} \overset{l'H}{=} \lim_{\omega\searrow 0} \frac{\varepsilon\left(1 - e^{-\varepsilon\omega}\right)^{-1} e^{-\varepsilon\omega}}{\varepsilon\left(e^{-\varepsilon\omega} - 1\right)^{-2} e^{-\varepsilon\omega}} = -\lim_{\omega\searrow 0}\left(1 - e^{-\varepsilon\omega}\right) = 0 \,,$$

(where "$l'H$" denotes the use of L'Hospital's rule) showing that these terms are bounded near $\omega = 0$. Next,

$$\lim_{\omega\to\infty} \frac{\log\left(1 - e^{-\varepsilon\omega}\right)}{e^{-\varepsilon\omega}} \overset{l'H}{=} \lim_{\omega\to\infty} \frac{\varepsilon\left(1 - e^{-\varepsilon\omega}\right)^{-1} e^{-\varepsilon\omega}}{-\varepsilon \, e^{-\varepsilon\omega}} = \lim_{\omega\to\infty} \frac{-1}{1 - e^{-\varepsilon\omega}} = -1 \,,$$

showing that as $\omega \to \infty$ those terms decay like $e^{-\varepsilon\omega}$. Therefore, these terms are also bounded and in $L^1(\mathbb{R})$. Now let $\kappa \neq 1$, then

$$\eta_\kappa\left(e^{-\varepsilon\omega}\right) = \log\left(e^{-\kappa\varepsilon\omega} + (1 - e^{-\varepsilon\omega})^\kappa\right) \,,$$

so the functions g_1 and g_2 are bounded. Moreover, $\eta_\kappa(e^{-\varepsilon\omega})$ decay like $e^{-\tilde{\kappa}\varepsilon\omega}$ with $\tilde{\kappa} := \min\{1, \kappa\}$ for $\omega \to \infty$ since

$$\lim_{\omega\to\infty} \left|\frac{\eta_\kappa\left(e^{-\varepsilon\omega}\right)}{e^{-\tilde{\kappa}\varepsilon\omega}}\right| \overset{l'H}{=} \frac{\kappa}{1 - \kappa} \lim_{\omega\to\infty} \left|\frac{\frac{e^{-(\kappa-1)\varepsilon\omega} - (1-e^{-\varepsilon\omega})^{\kappa-1}}{e^{-\kappa\varepsilon\omega} + (1-e^{-\varepsilon\omega})^\kappa}(-\varepsilon)e^{-\varepsilon\omega}}{-\varepsilon\varepsilon e^{-\tilde{\kappa}\varepsilon\omega}}\right|$$

$$= \frac{\kappa}{1 - \kappa} \lim_{\omega\to\infty} \left|\frac{\frac{e^{-\kappa\varepsilon\omega} - e^{-\varepsilon\omega}}{e^{-\kappa\varepsilon\omega} + 1}}{e^{-\tilde{\kappa}\varepsilon\omega}}\right| = \frac{\kappa}{1 - \kappa}$$

This shows that $\kappa \neq 1$; the functions g_1 and g_2 are in $L^1(\mathbb{R})$ as well.

7. Proof of the Main Result

We can now prove our main result.

Proof of Theorem 1.1. Having estimated all the error terms in trace norm and knowing that the limiting operator is trace class (see the proof of Theorem 5.7), we conclude that the operator

$$\eta_\kappa\big(\chi_\mathcal{K}\,(\Pi^\varepsilon_-)_{kn}\,\chi_\mathcal{K}\big) - \chi_\mathcal{K}\,\eta_\kappa\big((\Pi^\varepsilon_-)_{kn}\big)\,\chi_\mathcal{K}$$

is trace class. Moreover, we saw that all the error terms vanish after dividing by $\log \alpha$ and taking the limits $u_0 \to -\infty$ and $\alpha \to \infty$ (in this order). We thus obtain by Corollary 5.10,

$$\lim_{\alpha \to \infty} \lim_{u_0 \to -\infty} \frac{1}{\log \alpha}\Big(\eta_\kappa\big(\chi_\mathcal{K}\,(\Pi^\varepsilon_-)_{kn}\,\chi_\mathcal{K}\big) - \chi_\mathcal{K}\,\eta_\kappa\big((\Pi^\varepsilon_-)_{kn}\big)\,\chi_\mathcal{K}\Big)$$

$$= \lim_{\alpha \to \infty} \lim_{u_0 \to -\infty} \frac{1}{\log \alpha}\, \mathrm{tr}\, D_\alpha(\eta_\kappa, \mathcal{K}, \mathcal{A}_0) = \frac{1}{\pi^2} U(1; \eta_\kappa) = \frac{1}{\pi^2} \int_0^1 \frac{\eta_\kappa(t)}{t(1-t)}\, \mathrm{d}t\,.$$

Moreover, since by [23, Appendix],

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

and recalling that $\alpha = M/\varepsilon$, we obtain the result. □

8. Conclusions and Outlook

To summarize this article, we introduced the fermionic entanglement / Rényi entropy of a Schwarzschild black hole horizon based on the Dirac propagator as

$$S_\kappa^{\mathrm{BH}} = \frac{1}{2} \sum_{\substack{(k,n)\\ \text{occupied}}} \lim_{\varepsilon \searrow 0} \lim_{u_0 \to -\infty} \frac{1}{\log(M/\varepsilon)}\, \mathrm{tr}\Big(\eta_\kappa\big(\chi_\mathcal{K}(\Pi^\varepsilon_-)_{kn}\chi_\mathcal{K}\big) - \chi_\mathcal{K}\eta_\kappa\big((\Pi^\varepsilon_-)_{kn}\big)\chi_\mathcal{K}\Big).$$

$$(8.1)$$

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 $\mathcal{A}_0$ in (4.5) provided that $\kappa > \frac{2}{3}$. Since this symbol is diagonal matrix-valued, this reduces the problem to one spin dimension. Moreover, because $\mathcal{A}_0$ 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,

$$S_1^{\mathrm{BH}} = \sum_{\substack{(k,n) \\ \text{occupied}}} S_{1,kn}^{\mathrm{BH}} = \frac{1}{6} \, \#\big\{(k,n) \,\big|\, \text{angular mode } (k,n) \text{ occupied}\big\} \,,$$

and a similar result holds for the Rényi entropies with $\kappa > \frac{2}{3}$. This is comparable to the counting of states in string theory [35] and loop quantum gravity [1]. Furthermore, assuming that there is a minimal area of order ε^2, the number of occupied modes at the horizon was given by M^2/ε^2, which would lead to

$$S_1^{\mathrm{BH}} = \frac{1}{6} \, \frac{M^2}{\varepsilon^2} \,.$$

Bringing the factor $\log(M/\varepsilon)$ in (8.1) to the other side, this would mean that, up to lower orders in ε^{-1}, we would obtain the enhanced area law

$$\sum_{\substack{(k,n) \\ \text{occupied}}} \lim_{u_0 \to -\infty} \mathrm{tr} \, \Big(\eta_1 \big(\chi_{\mathcal{K}} (\Pi_-^\varepsilon)_{kn} \chi_{\mathcal{K}} \big) - \chi_{\mathcal{K}} \eta_1 \big((\Pi_-^\varepsilon)_{kn} \big) \chi_{\mathcal{K}} \Big)$$

$$= \frac{1}{6} \, \frac{M^2}{\varepsilon^2} \log(M/\varepsilon) + o\big(M^2/\varepsilon^2 \log(M/\varepsilon)\big) \,, \qquad \text{as } \varepsilon \searrow 0 \,. \tag{8.2}$$

One obvious question is whether this result holds not only in the Schwarzschild geometry, but for more general and physically realistic black holes. The core of our analysis makes use only of the asymptotic form of the Dirac wave functions near the event horizon. This leads to the conjecture that our results should hold for any black hole whose near-horizon geometry coincides with that of Schwarzschild. However, it is not clear to us how to prove this result, because our analysis is based on the integral representation of the Dirac propagator in [8], which holds only in the presence of global spacetime symmetries which allowing for the complete separation of the Dirac equation into a system of ordinary differential equations. We expect that the integral representation could be derived in general static and spherically symmetric black hole spacetimes, but this has not been worked out in the literature. Another generalization which seems possible from the perspective of separation of variables is the extension from Schwarzschild to the Kerr–Newman and 5D Myers–Perry family of rotating black holes, where corresponding integral representations have been derived (see [8,38]).

One another interesting topic for future research would be to analyze the number of occupied angular momentum modes at the horizon in more detail, in particular for a realistic model where the Schwarzschild black hole arises in the large time asymptotics of a spherically symmetric star undergoing gravitational collapse. Keeping into account the dynamical evolution of the regularization (as described, for example, by the regularized Hadamard expansion [10]), we do not expect that the resulting effective regularization length ε will be the same for each angular momentum mode. Therefore, the constant in (1.8) might

become n-dependent,

$$\lim_{\varepsilon \searrow 0} \lim_{u_0 \to -\infty} \frac{1}{\log(M/\varepsilon)} \operatorname{tr} \Delta_1\big((\Pi^\varepsilon_-)_{kn}, \mathcal{K}\big) = c(n) \,.$$

In this case, the counting of occupied states in (1.9) would have to be replaced by a weighted sum,

$$\sum_{(k,n) \text{ occupied}} c(n) \,.$$

This weighted sum can be understood as the effective number of occupied states. It might be that the weighted sum remains finite even if an infinite number of angular momentum modes (k, n) are taken into account.

Another interesting extension of our results is to consider more general quasi-free states in particular *thermal states*. Although our methods still apply in this situation, it is not clear to us which results to expect.

Finally, it seems possible to generalize our results technically as follows. Having mainly the von Neumann entropy function (i.e., $\kappa = 1$) in mind, we only established estimates for $R_\pm$ and its first derivative in u. This had the consequence that were not able to estimate the corresponding error terms for Rényi entropies with $\kappa \leq \frac{2}{3}$ with the same methods. However, those methods would also apply for $\kappa \leq \frac{2}{3}$ if one were able to estimate higher derivatives of $R_\pm$ suitably well. This is another topic for future research.

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Appendix A. A Few Technical Results on Pseudo-Differential Operators

Appendix provides a few technical results on pseudo-differential operators. By $\mathrm{Op}_\alpha(\mathcal{A})$, we always denote an operator as defined in Sect. 2.4.1.

Lemma A.1. *Let* $\mathrm{Op}_\alpha(\mathcal{A})$ *as defined in Sect. 3.3 with* $\mathcal{U} = \mathbb{R}^d$. *If the symbol* $\mathcal{A}$ *is hermitian matrix valued, measurable, independent of* $\boldsymbol{x}$ *and* $\boldsymbol{y}$, *i.e.,* $\mathcal{A}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\xi}) \equiv \mathcal{A}(\boldsymbol{\xi})$ *and is uniformly bounded in* $\boldsymbol{\xi}$ *(with respect to the ordinary matrix-sup-norm), then* $\mathrm{Op}_\alpha(\mathcal{A})$ *is well defined and self-adjoint. Moreover, for any Borel function* f *defined on the spectrum of* $\mathrm{Op}_\alpha(\mathcal{A})$, *we have*

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

Proof. Note that

$$\mathrm{Op}_\alpha(\mathcal{A}) = \mathcal{F} \, \mathcal{A}(./\alpha) \, \mathcal{F}^{-1} \, , \tag{A.1}$$

where $\mathcal{A}(./\alpha)$ denotes the matrix-multiplication operator by $\mathcal{A}(./\alpha)$ and $\mathcal{F}$ the unitary extension of the Fourier transform on $L^2(\mathbb{R}^d, C^n)$ (since (A.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 $\mathrm{Op}_\alpha(\mathcal{A})$ 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 $U(\boldsymbol{\xi})$ such that

$$U(\boldsymbol{\xi})\mathcal{A}(\boldsymbol{\xi}/\alpha)U(\boldsymbol{\xi})^{-1} = \mathrm{diag}(\mathfrak{d}_1(\boldsymbol{\xi}), \cdot, \mathfrak{d}_n(\boldsymbol{\xi})) =: \mathcal{D}(\boldsymbol{\xi}) \, .$$

Using the identification $L^2(\mathbb{R}^d, \mathbb{C}^n) \cong L^2(\{1, \ldots, n\} \times \mathbb{R}^d, \mathbb{C})$, the operator $U(\cdot)^{-1}\mathcal{F}^{-1}$ can be interpreted as the unitary transformation form the multiplicative version of the spectral theorem for the operator $\mathrm{Op}_\alpha(\mathcal{A})$ and $\mathcal{D}$ as the corresponding function.

Thus, we have

$$\begin{aligned} f(\mathrm{Op}_\alpha(\mathcal{A})) &= \mathcal{F} \, U(\cdot) \, f(\mathcal{D}(\cdot/\alpha)) \, U(\cdot)^{-1} \, \mathcal{F}^{-1} = \mathcal{F} \, f(\mathcal{A}(\cdot/\alpha)) \, \mathcal{F}^{-1} \\ &= \mathrm{Op}_\alpha(f(\mathcal{A})) \, . \end{aligned}$$

$\square$

Remark A.2. A similar argument as in the above proof can be used to prove a criterion on when the integral representation of $\mathrm{Op}_\alpha(\mathcal{A})$ extends to all Schwartz functions. Let $\mathcal{A}$ be a symbol which only depends on $\boldsymbol{x}$. Then, just as in the proof of Lemma A.1 we conclude that

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

Now take an arbitrary Schwartz function $\phi \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^n)$, then $\mathcal{F}\phi$ is defined with the usual integral representation. Moreover, since $\mathcal{F}$ is an automorphism on the Schwartz space $\mathcal{F}\phi \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^n)$. Furthermore, if the map $\mathcal{A}(\cdot/\alpha)(\mathcal{F}\phi)(\cdot)$ 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 $\mathrm{Op}_\alpha(\mathcal{A})$ extends to ϕ.

We conclude that if 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 $\mathrm{Op}_\alpha(\mathcal{A})$ extends to all Schwartz functions.

This is, for example, the case for any measurable and (in the matrix sup-norm) bounded symbol $\mathcal{A}$. $\diamondsuit$

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

Lemma A.3. *Let* $\mathrm{Op}_\alpha(\mathcal{A})$ *as in Sect.* 3.3, *let* $U, V \subset \mathbb{R}^d$ *be arbitrary Borel sets and* $\boldsymbol{c} \in \mathbb{R}^d$ *an arbitrary vector. For any* $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\xi} \in \mathbb{R}^d$ *we transform a given symbol* $\mathcal{A}$ *by*

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

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

$$t_{\boldsymbol{c}}\, \chi_{U+\boldsymbol{c}}\, \mathrm{Op}_\alpha\big(T_{-\boldsymbol{c}}(\mathcal{A})\big)\, \chi_{V+\boldsymbol{c}}\, t_{\boldsymbol{c}}^{-1} = \chi_U\, \mathrm{Op}_\alpha(\mathcal{A})\, \chi_V\,. \tag{A.2}$$

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

$$f\big(\chi_U\, \mathrm{Op}_\alpha(\mathcal{A})\, \chi_U\big) = t_{\boldsymbol{c}}\, f\big(\chi_{U+\boldsymbol{c}}\, \mathrm{op}_\alpha(T_{-\boldsymbol{c}}(\mathcal{A}))\, \chi_{U+\boldsymbol{c}}\big)\, t_{\boldsymbol{c}}^{-1}\,. \tag{A.3}$$

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

$$t_{\boldsymbol{c}} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d), \quad f \mapsto f(.\,+\boldsymbol{c})\,,$$

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

$$\chi_{W+\boldsymbol{c}} = t_{-\boldsymbol{c}}\, \chi_W\, t_{\boldsymbol{c}}\,,$$

and therefore

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

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

$$(t_{-\boldsymbol{c}}\, \mathrm{Op}_\alpha(\mathcal{A})\, t_{\boldsymbol{c}}\, \psi)(\boldsymbol{x})$$

$$= (\mathrm{Op}_\alpha(\mathcal{A})\, t_{\boldsymbol{c}}\, \psi)(\boldsymbol{x} - \boldsymbol{c}) = \frac{\alpha^d}{(2\pi)^d} \int \mathrm{d}\boldsymbol{\xi} \int \mathrm{d}\boldsymbol{y}\, e^{-i\alpha\boldsymbol{\xi}\,(\boldsymbol{x}-\boldsymbol{c}-\boldsymbol{y})}$$

$$\mathcal{A}(\boldsymbol{x} - \boldsymbol{c}, \boldsymbol{y}, \boldsymbol{\xi})\, \psi(\boldsymbol{y} + \boldsymbol{c})$$

$$= \frac{\alpha^d}{(2\pi)^d} \int \mathrm{d}\boldsymbol{\xi} \int \mathrm{d}\boldsymbol{y}\, e^{-i\alpha\boldsymbol{\xi}\,(\boldsymbol{x}-\boldsymbol{y})}\, \mathcal{A}(\boldsymbol{x} - \boldsymbol{c}, \boldsymbol{y} - \boldsymbol{c}, \boldsymbol{\xi},)\, \psi(\boldsymbol{y})$$

$$= (\mathrm{Op}_\alpha(T_{-\boldsymbol{c}}(\mathcal{A}))\psi)(\boldsymbol{x})\,.$$

This shows (A.2).

For (A.3), we make use of the multiplication operator version of the spectral theorem. This provides a unitary transformation ϕ and a suitable function g such that

$$\chi_U\, \mathrm{Op}_\alpha(\mathcal{A})\, \chi_U = \phi^{-1}\, g\, \phi\,.$$

Combined with the previous discussion, this implies

$$\chi_{U+\boldsymbol{c}}\, \mathrm{Op}_\alpha\big(T_{-\boldsymbol{c}}(\mathcal{A})\big)\, \chi_{U+\boldsymbol{c}} = (\phi\, t_{\boldsymbol{c}})^{-1}\, g\, (\phi\, t_{\boldsymbol{c}})\,,$$

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

$$
\begin{aligned}
f\big(\chi_{U+c}\, \mathrm{Op}_\alpha(T_{-c}(\mathcal{A}))\, \chi_{U+c}\big) &= (\phi\, t_c)^{-1}\, (f \circ g)\, (\phi\, t_c)\\
&= t_c^{-1}\, f\big(\chi_U\, \mathrm{Op}_\alpha(\mathcal{A})\, \chi_U\big)\, t_c\,,
\end{aligned}
$$

concluding the proof. $\hfill\square$

Remark A.4. A similar result as Lemma A.3 holds for translations in the $\boldsymbol{\xi}$-variable: Let $\boldsymbol{c} \in \mathbb{R}^d$ be an arbitrary vector. For any $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\xi} \in \mathbb{R}^d$ transform a given symbol $\mathcal{A}$ by

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

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

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

This shows that

$$
\mathrm{Op}_\alpha(R_{\boldsymbol{c}}(\mathcal{A})) = e^{i\alpha\boldsymbol{c}\cdot}\, \mathrm{Op}_\alpha(\mathcal{A})\, e^{-i\alpha\boldsymbol{c}\cdot}\,,
$$

which implies similar consequences for trace and Schatten norms since the operator $\mathcal{M}_{e^{i\alpha\boldsymbol{c}\cdot}}$ is unitary. $\hfill\Diamond$

Lemma A.5. *Let $\mathcal{A}$ be a symbol such that $\mathrm{Op}_\alpha(\mathcal{A})$ is well defined on $L^2(\mathbb{R}^d, \mathbb{C}^n)$, let $\mathcal{K} \subset \mathbb{R}$ be some measurable subset and $\alpha, \beta > 0$ some arbitrary constants. Then,*

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

$$
V_\beta^{-1}\, \chi_\mathcal{K}\, \mathrm{Op}_\alpha(\mathcal{A})\, \chi_\mathcal{K}\, V_\beta = \chi_{\beta\mathcal{K}}\, \mathrm{Op}_{\alpha/\beta}(\mathcal{A})\, \chi_{\beta\mathcal{K}}\,. \tag{A.4}
$$

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

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

$$
\mathrm{Op}_\alpha(\mathcal{A}) = \mathrm{Op}_{\beta\alpha}\big(\mathcal{A}(\beta\,\cdot)\big)\,. \tag{A.5}
$$

Proof. First, (ii) simply follows by changing coordinates in the $\boldsymbol{\xi}$-integral. For (i) consider the unitary operator V_β, which is for any $\psi \in L^2(\mathbb{R}^d, \mathbb{C}^n)$ defined by

$$
(V_\beta \varphi)(\boldsymbol{x}) := \beta^{d/2}\, \varphi(\beta\boldsymbol{x})\,, \qquad \text{for any } \boldsymbol{x} \in \mathbb{R}\,.
$$

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

$$
\big(V_\beta^{-1}\chi_\mathcal{K}V_\beta\psi\big)(\boldsymbol{x}) = \beta^{d/2}\big(V_\beta^{-1}\chi_\mathcal{K}\psi(\beta.)\big)(\boldsymbol{x}) = \chi_\mathcal{K}(x/\beta)\psi(\boldsymbol{x}) = \big(\chi_{\beta\mathcal{K}}\psi\big)(\boldsymbol{x})
$$

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

$$
\big(V_\beta^{-1}\mathrm{Op}_\alpha(\mathcal{A})V_\beta\psi\big)(\boldsymbol{x}) = \frac{\alpha^d}{2\pi} \int_{-\infty}^\infty \mathrm{d}\boldsymbol{\xi} \int_{-\infty}^\infty \mathrm{d}\boldsymbol{y}\, e^{i\alpha\boldsymbol{\xi}(x/\beta-\boldsymbol{y})} \mathcal{A}(\boldsymbol{\xi})\psi(\beta\boldsymbol{y})
$$

$$= \frac{(\alpha/\beta)^d}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\boldsymbol{\xi} \int_{-\infty}^{\infty} \mathrm{d}y \, e^{i\alpha/\beta\boldsymbol{\xi}(\boldsymbol{x}-\boldsymbol{y})} \mathcal{A}(\boldsymbol{\xi})\psi(\boldsymbol{y}) = (\mathrm{Op}_{\alpha/\beta}(\mathcal{A})\psi)(\boldsymbol{x}) \,,$$

where in the second step we applied a change of coordinates in the $\boldsymbol{y}$-integral.

$\square$

Lemma A.6. *Let* $\mathrm{Op}_\alpha(\mathcal{A})$ *as in Sect. 3.3, such that* $\mathcal{A}$ *satisfies*

$$\int_{\mathbb{R}^d} \mathrm{d}\boldsymbol{\xi} \sqrt{\int_{\mathcal{U}} \mathrm{d}\boldsymbol{y} \, \big\| \mathcal{A}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) \big\|_{n\times n}^2} < \infty \,, \qquad \textit{for any } \boldsymbol{x} \in \mathbb{R}^d$$

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

$$\Big(\mathrm{Op}_\alpha(\mathcal{A})\,\psi \Big)(\boldsymbol{x}) = \Big(\frac{\alpha}{2\pi}\Big)^d \int_{\mathbb{R}^d} \mathrm{d}\boldsymbol{\xi} \int_{\mathcal{U}} \mathrm{d}\boldsymbol{y} \, e^{-i\alpha\boldsymbol{\xi}\cdot(\boldsymbol{x}-\boldsymbol{y})} \, \mathcal{A}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) \, \psi(\boldsymbol{y})$$

$$= \Big(\frac{\alpha}{2\pi}\Big)^d \int_{\mathcal{U}} \mathrm{d}\boldsymbol{y} \int_{\mathbb{R}^d} \mathrm{d}\boldsymbol{\xi} \, e^{-i\alpha\boldsymbol{\xi}\cdot(\boldsymbol{x}-\boldsymbol{y})} \, \mathcal{A}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) \, \psi(\boldsymbol{y}) \,.$$

Proof. We first show that, applying the Fubini–Tonelli theorem and Hölder's inequality, the integrations may be interchanged, by estimating

$$\int_{\mathbb{R}^d} \mathrm{d}\boldsymbol{\xi} \int_{\mathcal{U}} \mathrm{d}\boldsymbol{y} \, \big| e^{-i\alpha\boldsymbol{\xi}\cdot(\boldsymbol{x}-\boldsymbol{y})} \mathcal{A}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi})\psi(\boldsymbol{y}) \big|$$

$$\leq \int_{\mathbb{R}^d} \mathrm{d}\boldsymbol{\xi} \, \sqrt{\int_{\mathcal{U}} \mathrm{d}\boldsymbol{y} \, \big\| \mathcal{A}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi})\psi(\boldsymbol{y}) \big\|_{n\times n}^2} \, \big\| \psi \big\|_{L^2(\mathbb{R}^d,\mathbb{C}^n)} < \infty \,.$$

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 $\big(\mathrm{Op}_\alpha(\mathcal{A})\psi \big)(\boldsymbol{x})$. 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 $\mathrm{Op}_\alpha(\mathcal{A})\psi$ is by definition given by

$$\mathrm{Op}_\alpha(\mathcal{A})\psi = \lim_{n\to\infty} \mathrm{Op}_\alpha(\mathcal{A})\psi_n \,, \tag{A.6}$$

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 $N \subseteq \mathbb{R}^d$. Moreover, for any $\boldsymbol{x} \in \mathcal{U}\backslash N$ and we can compute

$$\lim_{n\to\infty} \left| \Big(\frac{\alpha}{2\pi}\Big)^d \int_{\mathbb{R}^d} \mathrm{d}\boldsymbol{\xi} \int_{\mathcal{U}} \mathrm{d}\boldsymbol{y} \, e^{-i\alpha\boldsymbol{\xi}\cdot(\boldsymbol{x}-\boldsymbol{y})} \, \mathcal{A}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) \, \psi(\boldsymbol{y}) - \big(\mathrm{Op}_\alpha(\mathcal{A})\psi_n \big)(\boldsymbol{x}) \right|$$

$$= \lim_{n\to\infty} \left| \Big(\frac{\alpha}{2\pi}\Big)^d \int_{\mathbb{R}^d} \mathrm{d}\boldsymbol{\xi} \int_{\mathcal{U}} \mathrm{d}\boldsymbol{y} \, e^{-i\alpha\boldsymbol{\xi}\cdot(\boldsymbol{x}-\boldsymbol{y})} \, \mathcal{A}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) \, \Delta\psi_n(\boldsymbol{y}) \right|$$

$$\leq \Big(\frac{\alpha}{2\pi}\Big)^d \int_{\mathbb{R}^d} \mathrm{d}\boldsymbol{\xi} \, \sqrt{\int_{\mathbb{R}^d} \mathrm{d}\boldsymbol{y} \, \big\| \mathcal{A}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi}) \big\|_{n\times n}^2} \, \lim_{n\to\infty} \big\| \Delta\psi_n \big\|_{L^2(\mathbb{R}^d,\mathbb{C}^n)}^2 = 0 \,,$$

with $\Delta\psi_n := \psi - \psi_n$. Combining this estimate with the pointwise convergence (A.6) in $\mathcal{U} \backslash N$ yields the claim. $\square$

Remark A.7. We want to apply Lemma A.6 to the operator $\chi_{\mathcal{K}}(\Pi_-^\varepsilon)_{kn}\chi_{\mathcal{K}}$ with $\mathcal{K} = (u_0 - \rho, u_0)$. By rescaling as before, we see that this operator is of the form $\mathrm{Op}_\alpha(\mathcal{A}^{(\alpha)})$ with

$$\mathcal{A}^{(\alpha)}(u, u', \xi) = 2\,\chi_{\mathcal{K}}(u)\,\chi_{\mathcal{K}}(u')\,\chi_{(-\infty,0)}(\xi)\,e^{M\xi}$$
$$\times \sum_{a,b=1}^{2} t_{ab}^{kn(\alpha\xi)} \begin{pmatrix} X_{a,+}^{kn(\alpha\xi)}(u)\overline{X_{b,+}^{kn(\alpha\xi)}(u')} & X_{a,+}^{kn(\alpha\xi)}(u)\overline{X_{b,-}^{kn(\alpha\xi)}(u')} \\ X_{a,-}^{kn(\alpha\xi)}(u)\overline{X_{b,+}^{kn(\alpha\xi)}(u')} & X_{a,-}^{kn(\alpha\xi)}(u)\overline{X_{b,-}^{kn(\alpha\xi)}(u')} \end{pmatrix}.$$

Note that, apriori, the integral representation of this operator is well defined only for $C_0^\infty(\mathbb{R})^2$-functions with support in $\mathcal{K}$. In order to extend the integral representation to all $L^2(\mathcal{K}, \mathbb{C}^2)$-functions, it suffices to verify the condition in Lemma A.6. To this end, we note that, due to Lemma 2.3, for given $u_2 > u_0$, we have

$$|X_{a,i}^{kn(\alpha\xi)}(u)| < 1 + ce^{du},$$

for any $a \in \{1,2\}$, $i \in \{+,-\}$, $u < u_2$ and $\xi \in \mathbb{R}$, where the constants $c, d > 0$ are independent of ξ. Also using that the transmission coefficients t_{ab} are always bounded by $1/2$, we obtain the estimate

$$\|\mathcal{A}^{(\alpha)}(u, u`, \xi)\|_{n\times n} \leq C\,e^{M\xi}\,\chi_{(-\infty,0)}(\xi)\,\chi_{\mathcal{K}}(u)\,\chi_{\mathcal{K}}(u')$$

for any $\alpha > 0$ with C independent of u, u' and ξ. Thus, for any $u \in \mathcal{K}$ and $\alpha > 0$ we have

$$\int \mathrm{d}\xi \sqrt{\int \mathrm{d}u'\,\|\mathcal{A}^{(\alpha)}(u, u', \xi)\|_{n\times n}^2} = C \int_{-\infty}^{0} \mathrm{d}\xi \sqrt{\int_{u_0-\rho}^{u_0} \mathrm{d}u'\,e^{2M\xi}} = C\frac{\sqrt{\rho}}{M} < \infty.$$

Clearly, the entire expression vanishes for $u \notin \mathcal{K}$.

This shows that we can indeed apply Lemma A.6 to $\chi_{\mathcal{K}}(\Pi_-^\varepsilon)_{kn}\chi_{\mathcal{K}}$, meaning that the corresponding integral representation can be applied to any $L^2(\mathcal{K}, \mathbb{C}^2)$-function, and the u'- and ξ-integrations may be interchanged. Moreover, due to the characteristic functions in the symbol, we can even extend the integral representation to all functions in $L^2(\mathbb{R}, \mathbb{C}^2)$. $\Diamond$

Lemma A.8. *Let* $\mathcal{A}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\xi}) \equiv \mathcal{A}(\boldsymbol{x}, \boldsymbol{\xi})$ *(i.e., $\mathcal{A}$ is independent of $\boldsymbol{y}$) and* $\mathcal{B}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\xi}) \equiv \mathcal{B}(\boldsymbol{y}, \boldsymbol{\xi})$ *be symbols such that* $\mathrm{Op}_\alpha(\mathcal{A})$ *and* $\mathrm{Op}_\alpha(\mathcal{B})$ *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*

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

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*

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

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

Then

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

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

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

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 (where $\mathcal{F}$ is again the continuous extension of the Fourier transform to the Hilbert space $L^2(\mathbb{R}^d, \mathbb{C}^n)$). 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

$$\text{Op}_\alpha(\mathcal{A})\text{Op}_\alpha(\mathcal{B})\psi = AB\psi = \int_{\mathbb{R}^d} d\boldsymbol{\xi} \int_{\mathbb{R}^n} d\boldsymbol{x}\, e^{-i\alpha\boldsymbol{\xi}(\boldsymbol{x}-\boldsymbol{y})}\mathcal{A}(\boldsymbol{x}, \boldsymbol{\xi})\mathcal{B}(\boldsymbol{y}, \boldsymbol{\xi})\psi(\boldsymbol{y})\,.$$

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 $\text{Op}_\alpha(\mathcal{AB})$. □

Remark A.9.   (i) In what follows, we often apply the previous lemma in the case that

$$\mathcal{B}(\boldsymbol{y}, \boldsymbol{\xi}) = \chi_U(\boldsymbol{\xi})$$

for some measurable set $U \subseteq \mathbb{R}^d$. Then condition (ii) of Lemma A.8 is obviously fulfilled, because for any $\psi \in C_0^\infty(\mathbb{R}^d, \mathbb{C}^n)$ we have

$$B\psi = \chi_{\alpha U}\,\mathcal{F}^{-1}\psi\,,$$

and thus

$$\|B\psi\| = \|\chi_{\alpha U}\,\mathcal{F}^{-1}\psi\| \leq \|\mathcal{F}^{-1}\psi\| = \|\psi\|\,.$$

(ii) Moreover, in the following, the symbol $\mathcal{A}$ is sometimes independent of both $\boldsymbol{x}$ and $\boldsymbol{y}$ 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

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

and moreover,

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

Therefore, condition (i) in Lemma A.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

$$\text{supp}\,a \subseteq B_l(v) \times B_r(\mu)\,.$$

Then from the following argument we conclude that A also fulfills condition (i) from Lemma A.8. Take $\psi \in L^2(\mathbb{R}^d)$ arbitrary and consider

$$\int |A\psi(x)|^2 \, \mathrm{d}x$$

$$= \int_{B_l(v)} \mathrm{d}x \int_{B_r(\mu)} \mathrm{d}\xi \int_{B_r(\mu)} \mathrm{d}\xi' \, e^{-iu(\xi'-\xi)} \, \overline{\psi(\xi)} \, \psi(\xi') \, \overline{a(x,\xi/\alpha)} \, a(x,\xi'/\alpha)$$

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

$$\int_{B_l(v)} \mathrm{d}x \int_{B_r(\mu)} \mathrm{d}\xi \int_{B_r(\mu)} \mathrm{d}\xi' \, \left| \overline{\psi(\xi)} \, \psi(\xi') \, \overline{a(x,\xi/\alpha)} \, a(x,\xi'/\alpha) \right|$$

$$\leq C^2 \, \mathrm{vol}(B_l(v)) \, \|\psi\|^2_{L^1(B_r(\mu),\mathbb{C}^2)} < \infty \, ,$$

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

$$\int |A\psi(u)|^2 \, \mathrm{d}u$$

$$= \int \mathrm{d}\xi \, \overline{\psi(\xi)} \int \mathrm{d}\xi' \, \psi(\xi') \underbrace{\int \mathrm{d}x \, e^{-ix(\xi'-\xi)} \, \overline{a(x,\xi/\alpha)} \, a(x,\xi'/\alpha)}_{=:\tilde{a}(\xi,\xi')}$$

$$\leq \|\psi\| \int |\psi(\xi)| \, \|\tilde{a}(\xi,.)\| \, \mathrm{d}\xi \leq \|\psi\|^2 \sqrt{\int \mathrm{d}\xi \int \mathrm{d}\xi' \, |\tilde{a}(\xi,\xi')|^2} \, ,$$

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 A.8 is again satisfied. $\diamond$

Appendix B. Proof of Lemma 2.3

Proof. We follow the proof of [8, Lemma 3.1]. As explained there, employing the ansatz

$$X(u) = \begin{pmatrix} e^{-i\omega u} f^+(u) \\ e^{i\omega u} f^-(u) \end{pmatrix} , \tag{B.1}$$

the vector-valued function f must satisfy the ODE

$$\frac{\mathrm{d}}{\mathrm{d}u} f = \frac{\sqrt{\Delta(r)}}{r^2} \begin{pmatrix} 0 & e^{2i\omega u} \, (imr - \lambda) \\ e^{-2i\omega u} \, (-imr - \lambda) & 0 \end{pmatrix} f \, , \tag{B.2}$$

where λ is an eigenvalue of the operator

$$\mathcal{A} := \begin{pmatrix} 0 & \frac{\mathrm{d}}{\mathrm{d}\vartheta} + \frac{\cot \vartheta}{2} + \frac{k+1/2}{\sin \vartheta} \\ -\frac{\mathrm{d}}{\mathrm{d}\vartheta} - \frac{\cot \vartheta}{2} + \frac{k+1/2}{\sin \vartheta} & 0 \end{pmatrix}$$

(see [8, Appendix 1]) and thus does not depend on ω (in contrast with the Kerr–Newman case as explained in [8]). Estimating (B.2) gives

$$\left|\frac{\mathrm{d}}{\mathrm{d}u}f\right| \leq \left|\frac{\sqrt{r-2M}}{r^{3/2}}\right|(mr+|\lambda|)|f| = \sqrt{\frac{r-2M}{r}}\left(m+\frac{|\lambda|}{r}\right)|f| \,.$$

Next, we transform $r - 2M$ to the Regge–Wheeler coordinate,

$$r - 2M = 2M\, W\big(e^{u/(2M)-1}/2M\big) \,,$$

where W is the inverse log function, i.e., the inverse function of $x \mapsto xe^x$. An elementary estimate[3] shows that $W(x) \leq x$ for any $x \geq 0$, and therefore, we can estimate

$$\left|\frac{\mathrm{d}}{\mathrm{d}u}f\right| \leq \frac{e^{u/M-1/2}}{\sqrt{2M}}\left(m+\frac{|\lambda|}{2M}\right)|f| \,, \tag{B.3}$$

where we also used that $r \geq 2M$. Setting

$$c_1 := (2Me)^{-1/2}\left(m+\frac{|\lambda|}{2M}\right), \quad d := \frac{1}{M} \,,$$

we can proceed just as in [8, Proof of 3.1]:

Without loss of generality, we can assume that $|f|$ is nowhere vanishing[4] and divide (B.3) by $|f|$ giving

$$\frac{|\mathrm{d}/\mathrm{d}u f|}{|f|} \leq c_1 e^{\mathrm{d}u} \,.$$

This yields

$$\big|\log|f|(u_2) - \log|f|(u)\big| = \left|\int_u^{u_2}\frac{\frac{\mathrm{d}}{\mathrm{d}u}(|f^+|^2+|f^-|^2)}{|f|^2}\mathrm{d}u'\right| \leq 4\int_u^{u_2}c_1\,e^{\mathrm{d}u'}\,\mathrm{d}u'$$

$$= \frac{4c_1}{d}\big(e^{\mathrm{d}u_2} - e^{\mathrm{d}u}\big) \,.$$

From this, we conclude that

$$\log|f|(u) \geq \log|f|(u_2) - \frac{4c_1}{d}\big(e^{\mathrm{d}u_2} - e^{\mathrm{d}u}\big) \geq \log|f|(u_2) - \frac{4c_1}{d}e^{\mathrm{d}u_2}$$

$$\log|f|(u) \leq \log|f|(u_2) + \frac{4c_1}{d}\big(e^{\mathrm{d}u_2} - e^{\mathrm{d}u}\big) \leq \log|f|(u_2) + \frac{4c_1}{d}e^{\mathrm{d}u_2} \,,$$

which yields

$$|f(u_2)|\,\exp\Big(-\frac{4c_1}{d}e^{\mathrm{d}u_2}\Big) \leq |f(u)| \leq |f(u_2)|\,\exp\Big(\frac{4c_1}{d}e^{\mathrm{d}u_2}\Big) \,. \tag{B.4}$$

Using this inequality in (B.3), we obtain

$$\left|\frac{\mathrm{d}}{\mathrm{d}u}f\right| \leq c_1\,|f(u_2)|\,\exp\Big(\frac{4c_1}{d}e^{\mathrm{d}u_2}\Big)e^{\mathrm{d}u} \,, \tag{B.5}$$

---

[3]Since the function $f(x) := xe^x$ is strictly increasing (and differentiable) on $(0,\infty)$, so is $W = f^{-1}$ on $\big(f(0), f(\infty)\big) = (0,\infty)$. So from $xe^x \geq x$ for any $x \geq 0$ follows $x = W(xe^x) \geq W(x)$.
[4]If $|f(u)| = 0$ for one $u \in \mathbb{R}$, then due to (B.2) any order of derivative of f vanishes at u a and therefore, by the Picard–Lindelöf theorem, the function f vanishes identically on $\mathbb{R}$.

which shows that $\frac{\mathrm{d}f}{\mathrm{d}u}$ is integrable. Moreover, the function $f(u)$ converges for $u \to -\infty$ to

$$f_0 := \lim_{u \to -\infty} f(u) \overset{(B.4)}{\neq} 0 \,.$$

Now integrating (B.5) from $-\infty$ to $u < u_2$, we get

$$|f(u) - f_0| \leq \frac{c_1}{d} \, |f(u_2)| \, \exp\left(\frac{4c_1}{d} e^{\mathrm{d}u_2}\right) e^{\mathrm{d}u} \,. \tag{B.6}$$

Finally, in order to get rid of the factor $|f(u_2)|$, we make use of (B.4) in the limit $u \to -\infty$,

$$|f(u_2)| \leq |f_0| \, \exp\left(\frac{4c_1}{d} e^{\mathrm{d}u_2}\right) \,. \tag{B.7}$$

Substituting this in (B.6), we end up with the desired result

$$|f(u) - f_0| \leq c e^{\mathrm{d}u} \,,$$

with

$$c := \frac{c_1}{d} \, |f_0| \, \exp\left(\frac{8c_1}{d} e^{\mathrm{d}u_2}\right)$$

and

$$g(u) := f(u) - f_0 \,.$$

Similarly, removing $|f(u_2)|$ from (B.5) using (B.7) we obtain

$$\left|\frac{\mathrm{d}}{\mathrm{d}u} g\right| \leq d c e^{\mathrm{d}u} \,,$$

which completes the proof. $\qquad\square$

Appendix C. Computing the Symbol of $(\Pi_-^\varepsilon)_{kn}$

In this section, we give a more detailed computation of the symbol of the operator $(\Pi_-^\varepsilon)_{kn}$ for given k and n. Recall that $(\Pi_-^\varepsilon)_{kn}$ is for any function $\psi \in C_0^\infty(\mathbb{R}, \mathbb{C}^2)$ given by

$$\left((\Pi_-^\varepsilon)_{kn}\psi\right)(u) = \frac{1}{\pi} \int \mathrm{d}\omega \int \mathrm{d}u' e^{-\varepsilon\omega} \sum_{a,b=1}^{2} t_{a,b}^\omega X_a(u,\omega) \langle X_b(.,\omega) \, | \, \psi \rangle \,.$$

The main task is therefore to determine

$$\sum_{a,b=1}^{2} t_{a,b}^\omega X_a(u,\omega) X_b(u',\omega)^\dagger =: (*) \,. \tag{C.1}$$

To this end, first note that the details of the coefficients t_{ab} in (2.9) give

$$(*) = \chi_{(-m,0)}(\omega) \, X_1(u,\omega) \, X_1(u',\omega)^\dagger \tag{C.2}$$

$$+ \chi_{(-\infty,-m)}(\omega) \left[\frac{1}{2} \, X_1(u,\omega) \, X_1(u',\omega)^\dagger + \frac{1}{2} \, X_2(u,\omega) \, X_2(u',\omega)^\dagger \right. \tag{C.3}$$

$$\left. + t_{12}^\omega \, X_1(u,\omega) \, X_2(u',\omega)^\dagger + t_{21}^\omega \, X_2(u,\omega) \, X_1(u',\omega)^\dagger \right] \,. \tag{C.4}$$

Moreover, using the asymptotics of the radial solutions given in Lemma 2.3 the matrix $X_i(u,\omega)\,X_j(u',\omega)^\dagger$ can for any $i,j \in \{1,2\}$ be written as

$$X_i(u,\omega)\,X_j(u',\omega)^\dagger$$

$$= \begin{pmatrix} f_{0,i}^+(\omega)\,\overline{f_{0,j}^+(\omega)}\,e^{-i\omega(u-u')} & f_{0,i}^+(\omega)\,\overline{f_{0,j}^-(\omega)}\,e^{-i\omega(u+u')} \\ f_{0,i}^-(\omega)\overline{f_{0,j}^+(\omega)}\,e^{i\omega(u+u')} & f_{0,i}^-(\omega)\,\overline{f_{0,j}^-(\omega)}\,e^{i\omega(u-u')} \end{pmatrix} \tag{C.5}$$

$$+ R_{0,i}(u,\omega)\begin{pmatrix} f_{0,j}^+(\omega)\,e^{-i\omega u'} \\ f_{0,j}^-(\omega)\,e^{i\omega u'} \end{pmatrix}^\dagger + \begin{pmatrix} f_{0,i}^+(\omega)\,e^{-i\omega u} \\ f_{0,i}^-(\omega)\,e^{i\omega u} \end{pmatrix} R_{0,j}(u',\omega)^\dagger \tag{C.6}$$

$$+ R_{0,i}(u,\omega)\,R_{0,j}(u',\omega)^\dagger\,. \tag{C.7}$$

The terms in (C.6)-(C.7) will result in the error matrix $\mathcal{R}_0$ and are computed in Sect. 6.1.3. Here we are mainly interested in the terms in (C.5).

Combining our choices of f_0 from Sect. 2.3.4 with (C.5) and (C.2)-(C.4), we obtain

$$(*) = \chi_{(-m,0)}(\omega)\begin{pmatrix} |f_{0,1}^+(\omega)|^2\,e^{-i\omega(u-u')} & f_{0,1}^+(\omega)\,\overline{f_{0,1}^-(\omega)}\,e^{-i\omega(u+u')} \\ f_{0,1}^-(\omega)\overline{f_{0,1}^+(\omega)}\,e^{i\omega(u+u')} & |f_{0,1}^-(\omega)|^2\,e^{i\omega(u-u')} \end{pmatrix}$$

$$+ \chi_{(-\infty,-m)}(\omega)\begin{pmatrix} \frac{1}{2}\,e^{-i\omega(u-u')} & t_{12}^\omega\,e^{-i\omega(u+u')} \\ t_{21}^\omega\,e^{i\omega(u+u')} & \frac{1}{2}\,e^{i\omega(u-u')} \end{pmatrix} + \tilde{\mathcal{R}}_0(u,u',\omega)\,,$$

where $\tilde{\mathcal{R}}_0(u,u',\omega)$ consists of the terms (C.6)-(C.7) inserted in the sum (C.1).

In order to rewrite $(\Pi_-^\varepsilon)_{kn}$ 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 $\omega \to -\omega$ in the $d\omega$ integration of the $(2,2)$- and $(1,2)$-components. This yields (3.9).

Appendix D. Regularity of η_κ

We now verify in detail that the functions η_κ satisfy Condition 5.5.

Lemma D.1. *Consider the functions η_κ in (1.1). Then for any $\kappa \neq 1$, η_κ satisfies Condition 5.5 with $T = \{0,1\}$ for any $\gamma \leq \min\{1,\kappa\}$. Moreover, the function η_κ in (1.2) satisfies Condition 5.5 with $T = \{0,1\}$ for any $\gamma = \kappa$.*

Proof. We start with the case that $\kappa = 1$. Then,

$$\eta_1 \in C^2(\mathbb{R} \setminus \{0,1\}) \cap C^0(\mathbb{R})\,,$$

as

$$\lim_{t\to 0}\big(-t\log(t) - (1-t)\log(1-t)\big) = -\lim_{t\to 0}\frac{\log(t)}{t^{-1}} \overset{l'H}{=} \lim_{t\to 0}\frac{t^{-1}}{t^{-2}} = 0\,,$$

(where "$l'H$" denotes the use of l'Hospital's rule) and

$$\lim_{t\to 1}\big(-t\log(t) - (1-t)\log(1-t)\big) = -\lim_{t\to 1}\frac{\log(1-t)}{(1-t)^{-1}} \overset{l'H}{=}$$

$$-\lim_{t \to 1} \frac{(1-t)^{-1}}{(1-t)^{-2}} = 0 \,.$$

Moreover, for any $t \in (0,1)$ we have

$$\eta_1'(t) = -\log(t) + \log(1-t) \,,$$

$$\eta_1''(t) = -\frac{1}{t} - \frac{1}{1-t} \,.$$

Thus, for any $\gamma < 1$

$$\lim_{t \searrow 0} \eta_1(t) t^{-\gamma} = -\lim_{t \searrow 0} \frac{\log t}{t^{\gamma-1}} - \lim_{t \searrow 0} \frac{\log(1-t)}{t^\gamma} \overset{l'H}{=} -\lim_{t \searrow 0} \frac{t^{-1}}{(\gamma-1)t^{\gamma-2}}$$

$$+ \lim_{t \searrow 0} \frac{(1-t)^{-1}}{\gamma t^{\gamma-1}}$$

$$= \lim_{t \searrow 0} \frac{t^{1-\gamma}}{1-\gamma} + \lim_{t \searrow 0} \frac{t^{1-\gamma}}{\gamma(1-t)} = 0 \,,$$

and obviously

$$\lim_{t \nearrow 0} \eta_1(t) t^{-\gamma} = 0 \,.$$

Therefore, there exists a neighborhood $U_{0,0}$ of $z = 0$ and a constant $C_{0,0}$ such that for any $t \in U_{0,0}$,

$$|\eta_1(t)| \leq C_{0,0}|t|^\gamma \,.$$

Similarly,

$$\lim_{t \nearrow 1} \eta_1(t)(t-1)^{-\gamma} = \lim_{t \nearrow 1} \frac{\log t}{(1-t)^\gamma} + \lim_{t \nearrow 1} \frac{\log(1-t)}{(1-t)^{\gamma-1}}$$

$$\overset{l'H}{=} \lim_{t \nearrow 1} -\frac{t^{-1}}{\gamma(1-t)^{\gamma-1}} + \lim_{t \nearrow 1} \frac{(1-t)^{-1}}{(\gamma-1)(1-t)^{\gamma-2}} = 0 \,,$$

$$\lim_{t \searrow 1} \eta_1(t)(t-1)^{-\gamma} = 0 \,,$$

yielding a neighborhood $U_{1,0}$ of $z = 1$ and a constant $C_{1,0}$ such that for any $t \in U_{1,0}$:

$$|\eta_1(t)| \leq C_{1,0} |t-1|^\gamma \,.$$

The other estimates follow analogously by computing the limits

$$\lim_{t \searrow 0} \eta_1'(t) t^{1-\gamma} = -\lim_{t \searrow 0} \frac{\log(t)}{t^{\gamma-1}} \overset{l'H}{=} \lim_{t \searrow 0} \frac{t^{-1}}{(1-\gamma)t^{\gamma-2}} = \lim_{t \searrow 0} \frac{t^{1-\gamma}}{1-\gamma} = 0 \,,$$

$$\lim_{t \nearrow 1} \eta_1'(t)(t-1)^{1-\gamma} = -\lim_{t \nearrow 1} \frac{\log(1-t)}{(1-t)^{\gamma-1}} \overset{l'H}{=} \lim_{t \nearrow 1} \frac{(1-t)^{-1}}{(1-\gamma)(1-t)^{\gamma-2}}$$

$$= \lim_{t \nearrow 1} \frac{(1-t)^{1-\gamma}}{1-\gamma} = 0 \,,$$

$$\lim_{t \searrow 0} \eta_1''(t) t^{2-\gamma} = -\lim_{t \searrow 0} t^{1-\gamma} = 0 \,,$$

$$\lim_{t \nearrow 1} \eta_1''(t)(t-1)^{2-\gamma} = -\lim_{t \nearrow 1}(1-t)^{1-\gamma} = 0 \,,$$

$$\lim_{t \nearrow 0} \eta_1'(t) t^{1-\gamma} = \lim_{t \searrow 1} \eta_1'(t)(t-1)^{1-\gamma} = \lim_{t \nearrow 0} \eta_1''(t) t^{2-\gamma}$$
$$= \lim_{t \searrow 1} \eta_1''(t)(t-1)^{2-\gamma} = 0 \,.$$

This concludes the proof for the case that $\kappa = 1$.

Next, consider $\kappa \neq 1$. It is evident that

$$\eta_\kappa \in C^2(\mathbb{R} \setminus \{0,1\}) \cap C^0(\mathbb{R}) \,.$$

Moreover, the derivatives of η_κ for $t \in (0,1)$ are given by

$$\eta_\kappa'(t) = \frac{\kappa}{1-\kappa} \frac{t^{\kappa-1} - (1-t)^{\kappa-1}}{t^\kappa + (1-t)^\kappa} \,,$$

$$\eta_\kappa''(t) = \kappa \frac{t^{\kappa-2} + (1-t)^{\kappa-2}}{t^\kappa + (1-t)^\kappa} - \frac{\kappa^2}{1-\kappa} \frac{\left(t^{\kappa-1} + (1-t)^{\kappa-1}\right)^2}{t^\kappa + (1-t)^\kappa} \,.$$

Thus, we conclude that for $\kappa < 1$:

$$\eta_\kappa'(t) \simeq t^{\kappa-1} \,, \qquad \eta_\kappa''(t) \simeq t^{\kappa-2} \,, \qquad \text{for } t \searrow 0 \,,$$
$$\eta_\kappa'(t) \simeq (1-t)^{\kappa-1} \,, \qquad \eta_\kappa''(t) \simeq (1-t)^{\kappa-2} \,, \qquad \text{for } t \nearrow 1 \,,$$

so that we may choose $\gamma \leq \kappa$. For $1 < \kappa \leq 2$, first note that none of the first derivatives vanishes at $t = 0$ or $t = 1$, so we have

$$\eta_\kappa'(t) \simeq 1 \,, \qquad \eta_\kappa''(t) \simeq t^{\kappa-1} \,, \qquad \text{for } t \searrow 0 \,,$$
$$\eta_\kappa'(t) \simeq 1 \,, \qquad \eta_\kappa''(t) \simeq (1-t)^{\kappa-1} \,, \qquad \text{for } t \nearrow 1 \,,$$

and therefore, we can only take $\gamma \leq 1$. Similarly, for $\kappa > 2$ we have

$$\eta_\kappa'(t) \simeq 1 \,, \qquad \eta_\kappa''(t) \simeq 1 \,, \qquad \text{for } t \searrow 0 \,,$$
$$\eta_\kappa'(t) \simeq 1 \,, \qquad \eta_\kappa''(t) \simeq 1 \,, \qquad \text{for } t \nearrow 1 \,,$$

so we can only take $\gamma \leq 1$ as well. $\qquad\square$

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