TWO-TERM SPECTRAL ASYMPTOTICS FOR THE DIRICHLET PSEUDO-RELATIVISTIC KINETIC ENERGY OPERATOR ON A BOUNDED DOMAIN

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ABSTRACT. We consider the operator $A_m^\Omega := \sqrt{-\Delta+m^2}-m$ for $m>0$ with Dirichlet boundary condition on a bounded domain $\Omega\subset\mathbb{R}^d$ for $d\geqslant 2$. Continuing the long series of works following Hermann Weyl's famous one-term asymptotic formula for the counting function $N(\lambda)=\sum_{n=1}^\infty(\lambda_n-\lambda)_-^0$ of the eigenvalues of the Dirichlet Laplacian [54] and the much later found two-term expansion on domains with highly regular boundary by Ivriĭ [32] and Melrose [43], we prove a two-term asymptotic expansion of the N-th Cesàro mean of the eigenvalues of A_m^Ω as $N\to\infty$, generalizing a result by Frank and Geisinger [24] for the fractional Laplacian ($m=0$).

Until now, two-term asymptotic expansions for the eigenvalues of A_m^Ω have only been obtained for the heat trace $Z(t)=\sum_{n=1}^\infty e^{-t\lambda_n}$ (see Bañuelos et al. [6] and Park and Song [45]). Even though one can pass from heat trace asymptotics to one-term asymptotics of $N(\lambda)$ by using the Karamata Tauberian Theorem, this method cannot be used to obtain the subleading term in the expansion of $N(\lambda)$. However, large-N asymptotics of the Cesàro mean $\frac{1}{N}\sum_{n=1}^N\lambda_n$, and equivalently, large-λ asymptotics of the Riesz mean $R(\lambda):=\sum_{n=1}^\infty(\lambda_n-\lambda)_-$, is an intermediate step between heat trace and counting function asymptotics. In fact, $R(\lambda)$ can be obtained by integrating the counting function, while on the other hand, the heat trace can be obtained from the Laplace transform of $R(\lambda)$.

Large-λ asymptotics of $R(\lambda)$ is equivalent to small-h asymptotics of $\sum_{n=1}^\infty(h\lambda_n-1)_-$, which is the form in which we state our main result. We prove that, for all bounded domains $\Omega\subset\mathbb{R}^d$ with boundary $\partial\Omega\in C^1$ and for all $h,\mu>0$,

$$\operatorname{Tr}\big(hA_{\mu/h}^\Omega-1\big)_- \;=\; \Lambda_\mu^{(1)}\,|\Omega|\,h^{-d}-\Lambda_\mu^{(2)}\,|\partial\Omega|\,h^{-d+1}+R_\mu(h)\,, \qquad (*)$$

with $(1+\mu)^{-d/2}R_\mu(h)\in o(h^{-d+1})$ uniformly in $\mu>0$, as $h\to 0$. In the case $\partial\Omega\in C^{1,\gamma}$ for some $\gamma>0$, we obtain a slightly better remainder estimate. Here, $|\Omega|$ denotes the volume of the domain, $|\partial\Omega|$ its surface area, $\Lambda_\mu^{(1)}$ the Weyl constant for A_μ^Ω, and $\Lambda_\mu^{(2)}$ is given in terms of an explicit diagonalization of a family of one-dimensional model operators on the half-line due to Kwaśnicki [37]. We derive a two-term formula for the small-h asymptotics of $\sum_{n=1}^\infty(h\lambda_n-1)_-$ by applying $(*)$ with $\mu=hm$, extending the case $s=\frac{1}{2}$ in [24] to A_m^Ω with $m>0$ and improving the earlier results [6] and [45] for $Z(t)$.

SPEKTRALE ZWEI-TERM-ASYMPTOTIK FÜR DEN PSEUDO-RELATIVISTISCHEN KINETISCHEN ENERGIE-OPERATOR AUF EINEM BESCHRÄNKTEN GEBIET

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Zusammenfassung. Wir betrachten den Operator $A_m^\Omega := \sqrt{-\Delta + m^2} - m$ für $m > 0$ mit Dirichlet-Randbedingung auf einem beschränkten Gebiet $\Omega \subset \mathbb{R}^d$ für $d \geqslant 2$ und setzen die lange Serie von Arbeiten fort, die auf Hermann Weyls berühmte Ein-Term-Asymptotik der Zählfunktion $N(\lambda) = \sum_{n=1}^\infty (\lambda_n - \lambda)_-^0$ für die Eigenwerte des Dirchlet Laplace-Operators [54] und die einige Zeit später bewiesene Zwei-Term-Entwicklung für Gebiete mit hoher Rand-Regularität durch Ivriĭ [32] und Melrose [43], gefolgt sind. Wir beweisen eine Zwei-Term-Asymptotik für das Nte Cesàro-Mittel der Eigenwerte von A_m^Ω für $N \to \infty$ und verallgemeinern dadurch ein Resultat von Frank und Geisinger [24] für den fraktionellen Laplace-Operator ($m = 0$).

Bis jetzt wurden Zwei-Term-Asymptotiken für die Eigenwerte von A_m^Ω nur für die Spur des Wärmeleitungskerns $Z(t) = \sum_{n=1}^\infty e^{-t\lambda_n}$ bewiesen (siehe Bañuelos et al. [6] sowie Park und Song [45]). Obwohl man mithilfe des Tauberischen Theorems von Karamata den ersten Term in der Groß-λ-Asymptotik von $N(\lambda)$ aus der Klein-t-Asymptotik von $Z(t)$ erhält, kann diese Methode nicht verwendet werden um, den zweiten Term in der Asymptotik von $N(\lambda)$ zu finden. Die Groß-N-Asymptotik des Cesàro-Mittels $\frac{1}{N}\sum_{n=1}^N \lambda_n$ hingegen, sowie äquivalent dazu die Groß-λ-Asymptotik des Riesz-Mittels $R(\lambda) := \sum_{n=1}^\infty (\lambda_n - \lambda)_-$, kann als Zwischenschritt der Asymptotiken von $N(\lambda)$ und $Z(t)$ gesehen werden. In der Tat erhält man $R(\lambda)$ aus der Integration von $N(\lambda)$, während $Z(t)$ aus der Laplace-Transformierten von $R(\lambda)$ gewonnen werden kann.

Die Asymptotik von $R(\lambda)$ für $\lambda \to \infty$ ist äquivalent zur Asymptotik von $\sum_{n=1}^\infty (h\lambda_n - 1)_-$ für $h \to 0^+$, und dies ist die Form in der wir unser Hauptresultat formulieren. Wir beweisen, dass für alle beschränkten Gebiete $\Omega \subset \mathbb{R}^d$ mit $\partial\Omega \in C^1$ und für alle $h, \mu > 0$ gilt

$$\operatorname{Tr}\big(hA_{\mu/h}^\Omega - 1\big)_- = \Lambda_\mu^{(1)} |\Omega| \, h^{-d} - \Lambda_\mu^{(2)} |\partial\Omega| \, h^{-d+1} + R_\mu(h) \,, \qquad (*)$$

mit $(1+\mu)^{-d/2} R_\mu(h) \in o(h^{-d+1})$, gleichmäßig in $\mu > 0$ für $h \to 0$. Im Falle von $\partial\Omega \in C^{1,\gamma}$ für $\gamma > 0$ erhalten wir eine geringfügig bessere Restterm-Abschätzung. Hier gibt $|\Omega|$ das Volumen des Gebiets und $|\partial\Omega|$ dessen Oberflächeninhalt an, $\Lambda_\mu^{(1)}$ ist die Weyl-Konstante für A_μ^Ω und $\Lambda_\mu^{(2)}$ ist mithilfe einer expliziten Diagonalisierung einer Familie von eindimensionalen Modell-Operatoren auf der Halbachse (siehe Kwaśnicki [37]) gegeben. Schließlich leiten wir eine Zwei-Term-Formel für die Klein-h-Asymptotik von $\sum_{n=1}^\infty (h\lambda_n - 1)_-$ her, indem wir $(*)$ mit $\mu = hm$ anwenden. So erweitern wir den Fall $s = \frac{1}{2}$ in [24] auf A_m^Ω mit $m > 0$ und verbessern die früheren Resultate [6] und [45] für $Z(t)$.

Contents

Introduction and main results

Introduction. Let $d \in \mathbb{N}$ and let $\Omega \subset \mathbb{R}^d$ be open. For $m \geqslant 0$, let $A_m^\Omega = (\sqrt{-\Delta+m^2}-m)_D$ denote the self-adjoint operator in $L^2(\mathbb{R}^d)$ defined by the closed quadratic form

$$q_m^\Omega(u) = \int_{\mathbb{R}^d} \big(\sqrt{|2\pi\xi|^2 + m^2} - m\big)\, |\hat{u}(\xi)|^2 \, d\xi \tag{0.1}$$

with form domain $\mathcal{D}(q_m^\Omega) = H_0^{1/2}(\Omega)$ (see Appendix A for a short overview of fractional Sobolev spaces). Here $\hat{u}$ denotes the Fourier transform[1] of u.

If Ω is bounded, then A_m^Ω has compact resolvent, since the embedding $H_0^{1/2}(\Omega) \hookrightarrow L^2(\Omega)$ is compact (see Appendix A). In particular, its spectrum consists of eigenvalues[2]

$$0 < \lambda_1 < \lambda_2 \leqslant \lambda_3 \leqslant \cdots , \tag{0.2}$$

accumulating at infinity only.

As discovered by Hermann Weyl in 1912, there is an explicit connection between the asymptotic growth of the counting function $N(\lambda) := \sum_n (\lambda_n - \lambda)_-^0$ for the eigenvalues λ_n of the Dirichlet Laplacian $(-\Delta)_D$ and geometric properties of the domain. More precisely, by his celebrated result [54], for $(-\Delta)_D$ on a domain Ω with piecewise smooth boundary, we have

$$N(\lambda) \,=\, C^{(1)}\, |\Omega|\, \lambda^{d/2} + o(\lambda^{d/2}) \ , \quad \text{as } \lambda \to \infty \,, \tag{0.3}$$

where $C^{(1)} := (2\pi)^{-d}\, \omega_d$ with ω_d denoting the volume of the d-dimensional unit ball. Based on so called Tauberian theorems (see [30], [55, p. 192], or [20, p. 445]), Weyl's Law has been extended to domains with less regularity by methods due to Carleman [11] and Gårding [27].

In 1913, Weyl conjectured the second term in the asymptotic expansion (0.3) to be of the form $-C\, \lambda^{(d-1)/2}$, with a positive constant C that is proportional to the surface area $|\partial\Omega|$ of the boundary (originally just in two dimensions; see [12]). Only in 1980, V. Ivriĭ confirmed Weyl's conjecture by methods from microlocal analysis. Under the additional assumption that the measure of the set of all periodic billiard trajectories is zero, he proved in [32] for $(-\Delta)_D$ on domains with smooth boundary, that

$$N(\lambda) \,=\, C^{(1)}\, |\Omega|\, \lambda^{d/2} - C^{(2)}\, |\partial\Omega|\, \lambda^{(d-1)/2} + o(\lambda^{(d-1)/2}), \ \text{as } \lambda \to \infty, \tag{0.4}$$

where $C^{(2)} = \frac{1}{4}(2\pi)^{-d+1}\, \omega_{d-1}$. In the same year, R. B. Melrose proved an analogous result for compact Riemannian manifolds with convex boundary under additional assumptions on the relation between the boundary and the geodesic flow (see [43]). His proof is based on methods used earlier by Babic and Levitan [4], Hörmander [31], Duistermaat and Guillemin [16], and Seeley [49]. Prior to the results of Ivriĭ and Melrose, improvements to the remainder in Weyl's law (0.3) have been obtained by many authors, including Courant [13], Hörmander [31], Brüning [10], Babic and Levitan [4], and Seeley [49].

The dependency on geometric quantities, like the volume and surface area, is not a unique feature of the large-λ asymptotics of $N(\lambda)$, but is shared with the asymptotic expansions of other functions of the eigenvalues, such as small-time asymptotics of the heat trace

$$Z(t) = \sum_{n=1}^{\infty} e^{-t\lambda_n} = D^{(1)} |\Omega|\, t^{-d/2} - D^{(2)} |\partial\Omega|\, t^{-(d-1)/2} + o(t^{-(d-1)/2}) \quad \text{as } t \to 0^+, \tag{0.5}$$

[1] We use the convention $\hat{f}(\xi) = \mathcal{F}f(\xi) = \int_{\mathbb{R}^d} e^{-2\pi i \xi x} f(x) dx$ for any $f \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$.

[2] Non-degeneracy of the ground state follows from a Perron-Frobenius-type argument, see e.g. [46, XIII.12].

where $D^{(1)}$ and $D^{(2)}$ are positive constants only depending on the dimension, or large-λ asymptotics of the Riesz mean $R(\lambda) = \sum_{n=1}^{\infty}(\lambda_n - \lambda)_-$ (see (0.8) below). While (0.5) had been known for several classes of domains before[3], it was proved by R. M. Brown in [9] for Lipschitz domains. Heuristically, $Z(t)$ for $t > 0$ can be considered as a regularization of $\lim_{\lambda\to\infty} N(\lambda)(= Z(0^+))$, which formally justifies the asymptotic similarities of $Z(t)$ and $N(\lambda)$. Rigorously, as was first noted by M. Kac in his classic article *Can one hear the shape of a drum?* [35], Weyl's law (0.3) can be recovered from the first term in (0.5) by using the Karamata Tauberian Theorem [55, p. 192]. In addition to extending Weyl's Law to less regular domains (as in [9]), this allows to deduce one-term expansions of $N(\lambda)$ for other operators than $(-\Delta)_D$, for which corresponding heat trace asymptotics are available.

In this way, based on their asymptotic results on Markov operators [7], Blumenthal and Getoor proved in [8] for the fractional Laplacian $((-\Delta)^{\alpha/2})_D$, $\alpha \in (0, 2]$, on domains Ω with boundaries that have zero d-dimensional Lebesgue measure (e.g. Lipschitz domains), that

$$N(\lambda) = C_\alpha^{(1)}\,|\Omega|\,\lambda^{d/\alpha} + o(\lambda^{d/\alpha}), \qquad \text{as } \lambda \to \infty\,, \tag{0.6}$$

where $C_\alpha^{(1)} = 2^d\,\pi^{d/2}\,\Gamma(d/\alpha{+}1)$.

The fractional analogue of (0.5), which is due to Bañuelos et al. [5], has recently been extended to $((-\Delta{+}m^{2/\alpha})^{\alpha/2}{-}m)_D$ by Park and Song [45]. They prove for Lipschitz domains[4], that

$$Z(t) = D_\alpha^{(1)}\,|\Omega|\,t^{-d/\alpha} - (D_\alpha^{(2)}\,|\partial\Omega| - m\,D_\alpha^{(3)}\,|\Omega|)\,t^{-(d-1)/\alpha} + o(t^{-(d-1)/\alpha}) \qquad \text{as } t \to 0^+, \tag{0.7}$$

where $D_\alpha^{(1)}, D_\alpha^{(2)}$ and $D_\alpha^{(3)}$ are positive constants only depending on $\alpha \in (0, 2]$ and $d \geqslant 2$. In particular, this shows that the leading term in the asymptotics of $Z(t)$, and hence also $N(\lambda)$, does not depend on m.

In general, asymptotic formulas for $Z(t)$ (the sum of the *smooth* functions $t \mapsto e^{-t\lambda_n}$) are usually more detailed and known for more general domains than those for $N(\lambda)$. From this point of view, the result [24] by R. L. Frank and L. Geisinger can be seen as an intermediate step between heat trace and counting function asymptotics. They prove a two-term asymptotic expansion of the N-th Cesàro mean $\frac{1}{N}\sum_{j=1}^{N}\lambda_j$ as $N \to \infty$ for $((-\Delta)^{\alpha/2})_D$ on C^1 domains[5]. More precisely, they prove the equivalent result for the Riesz mean $R(\lambda)$,

$$\sum_{n=1}^{\infty}\big(\lambda_n{-}\lambda\big)_- \;=\; L_\alpha^{(1)}|\Omega|\,\lambda^{1+d/\alpha} - L_\alpha^{(2)}|\partial\Omega|\lambda^{1+(d-1)/\alpha} + o(\lambda^{1+(d-1)/\alpha}) \;\text{ as } \lambda \to \infty\,, \tag{0.8}$$

where $L_\alpha^{(1)}$ and $L_\alpha^{(2)}$ are positive constants only depending on $\alpha \in (0, 2]$ and $d \geqslant 2$. This is an improvement of the corresponding heat trace asymptotics to the sum of the less regular functions $\lambda \mapsto (\lambda_n{-}\lambda)_-$. In fact, this is a step in between the asymptotics of $Z(t)$ and $N(\lambda)$, since $R(\lambda)$ can be obtained by integrating $N(\lambda)$, while on the other hand, $Z(t)$ can be obtained from the Laplace transform of $R(\lambda)$ (see (0.19) below).

[3] For example, for plane polygonal regions it is due to Kac [35], for manifolds with compact boundary it is due to McKean and Singer [42], for compact domains with smooth boundary it is due to Greiner [28], and for convex domains with bounded curvature it is due to van den Berg [53].

[4] For domains with $C^{1,1}$ boundary, they can improve the remainder to $\mathcal{O}(t^{-(d-2)/\alpha})$.

[5] In [24], the asymptotic formula (0.8) is proved for $C^{1,\gamma}$ domains, for any $0 < \gamma \leqslant 1$, with a remainder whose order depends on γ. But, as noted in [21], the stated result follows for C^1 domains by the same argument as in [23] (see also proof of our Theorem 1 in Section 8).

In this work, we will extend the case $\alpha = 1$ of (0.8), i.e. the large-λ asymptotics of $R(\lambda)$ for the eigenvalues of $A_0^\Omega = (\sqrt{-\Delta})_D$, to $A_m^\Omega = (\sqrt{-\Delta+m^2}-m)_D$ for $m > 0$. The most notable difference to the massless case is the fact that

$$\psi_m(|\xi|^2) := \sqrt{|\xi|^2 + m^2} - m \tag{0.9}$$

fails to be homogeneous in $\xi \in \mathbb{R}^d$. Thus, even though the overall structure of the proof is similar to [24], the lack of homogeneity often requires to change the techniques used in [24] or to approach problems differently. One of the key tools we use to overcome these difficulties is the integral representation,

$$q_m^\Omega(u) \;=\; \Big(\frac{m}{2\pi}\Big)^{(d+1)/2} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} |u(x){-}u(y)|^2\, \frac{K_{(d+1)/2}(m|x{-}y|)}{|x{-}y|^{(d+1)/2}}\, dx\, dy \tag{0.10}$$

for all $u \in H_0^{1/2}(\Omega)$, where K_β denotes the Modified Bessel Function of the Second Kind of order β (see Appendix D.2). Equation (0.10) follows from the corresponding integral representation of the kernel of $e^{-tA_m^\Omega}$ (see (E.28)). In Appendix E.7, we derive (0.10) by using results from probability theory.

Statement and consequences of the main theorem. Due to the inhomogeneity of ψ_m, the statement of Theorem 1 involves a new parameter $\mu > 0$. In order to obtain an asymptotic expansion of $\sum_{n\in\mathbb{N}}(h\lambda_n{-}1)_-$ as $h \to 0$ for the eigenvalues of A_m^Ω, we apply Theorem 1 with $\mu = hm$ in Theorem 2 below.

Theorem 1. *For $h, \mu > 0$, $d \geqslant 2$, and a bounded open subset $\Omega \subset \mathbb{R}^d$, let $H_{\mu,h}^\Omega := h\,A_{\mu/h}^\Omega - 1$ with Dirichlet boundary condition on Ω, i.e. $H_{\mu,h}^\Omega = (\sqrt{-h^2\Delta{+}\mu^2}-\mu-1)_D$. If the boundary $\partial\Omega$ belongs to C^1, then for all $h, \mu > 0$,*

$$\operatorname{Tr}\big(H_{\mu,h}^\Omega\big)_- \;=\; \Lambda_\mu^{(1)}\, |\Omega|\, h^{-d} - \Lambda_\mu^{(2)}\, |\partial\Omega|\, h^{-d+1} + R_\mu(h)\,, \tag{0.11}$$

with $(1{+}\mu)^{-d/2} R_\mu(h) \in o(h^{-d+1})$ uniformly in $\mu > 0$, as $h \to 0^+$.

In the case when $\partial\Omega$ belongs to $C^{1,\gamma}$ for some $\gamma > 0$, then for all $\varepsilon \in (0, \gamma/(\gamma{+}2))$, there exists $C_\varepsilon(\Omega) > 0$ such that for all $h, \mu > 0$, $|R_\mu(h)| \leqslant C_\varepsilon(\Omega)\,(1{+}\mu)^{d/2}\, h^{-d+1+\varepsilon}$.

Here, $|\Omega|$ denotes the volume of the domain and $|\partial\Omega|$ its surface area. Moreover,

$$\Lambda_\mu^{(1)} := \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \Big(\sqrt{|\xi|^2{+}\mu^2} - \mu - 1\Big)_- d\xi \tag{0.12}$$

and

$$\Lambda_\mu^{(2)} \;:=\; \frac{1}{(2\pi)^d}\int_0^\infty \int_{\mathbb{R}^d} \Big(\sqrt{|\xi|^2{+}\mu^2} - \mu - 1\Big)_- \Big(1{-}2F_{\mu/|\xi'|,|\xi_d|/|\xi'|}(|\xi'|t)^2\Big)\, d\xi\, dt\,, \tag{0.13}$$

where $\xi' = (\xi_1, \ldots, \xi_{d-1})$, and, for $\omega \geqslant 0$, $F_{\omega,\lambda}$ are the generalized eigenfunctions of the one-dimensional operator $(\sqrt{-d^2/dt^2{+}1{+}\omega^2} - \sqrt{1{+}\omega^2})_D$ with Dirichlet boundary condition on the half-line, given by Kwaśnicki in [37].

In order to apply Theorem 1 with $\mu = hm$ in Theorem 2 below, we compare the constants in (0.11) with their counterparts for $\mu = 0$. An explicit computation shows that there exists $C > 0$, such that for all $\mu > 0$

$$\Big|\Lambda_\mu^{(1)} - \Lambda_0^{(1)} - \tfrac{\omega_d}{(2\pi)^d}\,\mu\Big| \;\leqslant\; C\,\mu^2\,, \tag{0.14}$$

where $\Lambda_0^{(1)} = (2\pi)^{-d}\int_{\mathbb{R}^d}(|p|-1)_- dp = (2\pi)^{-d}(d+1)^{-1}\omega_d$ is the corresponding Weyl constant for $(\sqrt{-\Delta})_D$. Similarly, by a detailed analysis of the generalized eigenfunctions $F_{\omega,\lambda}$ (see Appendix F.1), for $d \geqslant 2$ and any $\delta \in (0,1)$, there exists $C_\delta > 0$, such that for all $\mu > 0$,

$$\left|\Lambda_\mu^{(2)} - \Lambda_0^{(2)}\right| \;\leqslant\; C_\delta\,\mu^\delta\,, \tag{0.15}$$

where $\Lambda_0^{(2)} = L_1^{(2)} > 0$ denotes the second constant in (0.8) for $(\sqrt{-\Delta})_D$.

As a consequence, we obtain

Theorem 2. *For $m \geqslant 0$, $d \geqslant 2$, $n \in \mathbb{N}$, and a bounded open subset $\Omega \subset \mathbb{R}^d$ let λ_n denote the n-th eigenvalue of $A_m^\Omega = (\sqrt{-\Delta + m^2} - m)_D$. In the case when $\partial\Omega$ belongs to C^1, then for all $h > 0$,*

$$\sum_{n\in\mathbb{N}} \big(h\lambda_n - 1\big)_- \;=\; \Lambda_0^{(1)}\,|\Omega|\,h^{-d} - \Big(\Lambda_0^{(2)}|\partial\Omega| - C_d\,|\Omega|\,m\Big)\,h^{-d+1} + r_m(h)\,, \tag{0.16}$$

with $(m^\delta + m^2 + (1+m)^{d/2})^{-1} r_m(h) \in o(h^{-d+1})\ \forall\delta > 0$, uniformly in $m > 0$, as $h \to 0^+$.

In the case when $\partial\Omega$ belongs to $C^{1,\gamma}$ for some $\gamma > 0$, then for each $\varepsilon \in (0, \gamma/(\gamma+2))$ there exists $C_\varepsilon(\Omega) > 0$ such that

$$|r_m(h)| \leqslant C_\varepsilon(\Omega)\,\big(m^\varepsilon + m^2 + (1+mh)^{d/2}\big)\,h^{-d+1+\varepsilon}\,.$$

Here, $C_d := \frac{\omega_d}{(2\pi)^d}$, $\Lambda_0^{(1)} = \frac{C_d}{d+1}$, and $\Lambda_0^{(2)}$ is given in (0.13) and coincides with $L_1^{(2)}$, the second constant in (0.8) for $\alpha = 1$.

This follows immediately from Theorem 1 by substituting $\mu = hm$ and using the inequalities (0.14) and (0.15) (see Section 8).

Structure of the proof of Theorem 1. Following [51], [50], and [24], in Section 1, we construct a family of localization functions $\{\phi_u\}_{u\in\mathbb{R}^d} \subset C_0^1(\mathbb{R}^d)$, such that ϕ_u is supported in a ball of radius $l(u)$, where $l : \mathbb{R}^d \to [0,\infty)$ is an increasing function of the distance to the complement Ω^c, satisfying $\frac{l_0}{3} < l(u) < \frac{1}{2}$ for a given parameter $l_0 \in (0, \frac{1}{2})$, and[6]

$$\int_{\mathbb{R}^d} \phi_u(x)^2\, l(u)^{-d} du = 1 \quad \forall x \in \mathbb{R}^d\,. \tag{1.4}$$

In this sense, $\{\phi_u\}_{u\in\mathbb{R}^d}$ can be thought of as a partition of unity with respect to the continuous parameter u. In fact, (1.4) implies an IMS-type localization formula (Lemma 6) that allows to write $\mathrm{Tr}(H_{\mu,h}^\Omega)_-$ in terms of $\mathrm{Tr}\big(\phi_u H_{\mu,h}^\Omega \phi_u\big)_-$, at the expense of an error term, which has an upper bound with explicit depency on h, μ and l_0 (see Proposition 5). The general idea of this approach is due to [40] and [51].

From here, it remains to study $\mathrm{Tr}\big(\phi H_{\mu/h}^\Omega \phi\big)_-$, separately for ϕ with support completely contained Ω (in the *bulk*) and with support in a ball intersecting the boundary of Ω.

In the case when the support of ϕ is completely contained in Ω, we have $\phi f \in H_0^{1/2}(\Omega)$ for all $f \in H_0^{1/2}(\mathbb{R}^d)$. Thus, in Section 2, we compare $\mathrm{Tr}\big(\phi H_{\mu,h}^\Omega \phi\big)_-$ with the upper bound

$$\mathrm{Tr}\big(\phi H_{\mu,h}^\Omega \phi\big)_- \;\leqslant\; \mathrm{Tr}\,\phi\big(H_{\mu,h}^{\mathbb{R}^d}\big)_-\phi \;=\; \Lambda_\mu^{(1)}\,h^{-d}\int_{\mathbb{R}^d}\phi(x)^2\,dx\,, \tag{2.2}$$

[6] Here, the numbering of the equations refers to the actual numbers in the main body of the thesis where they are situated.

and obtain an error explicitly depending on h, μ and l_ϕ, where l_ϕ is the radius of a ball containing the support of ϕ (see Proposition 8). The proof is based on the representation

$$\big\|(h A_{\mu/h})^{1/2}\phi e^{ip\cdot/h}\big\|_2^2 \,=\, \frac{1}{2}\int_{\mathbb{R}^d} \big(\psi_\mu(|p{+}2\pi h\eta|^2) + \psi_\mu(|p{-}2\pi h\eta|^2)\big)\, |\hat{\phi}(\eta)|^2\, d\eta\,, \tag{2.4}$$

shown in Lemma 10, and, besides technical details, it follows along the same lines as the proof of [24, Prop. 4].

In Section 3, we perform what is known as *straightening of the boundary*, which means that we use the assumption that the boundary is locally given by the graph of a differentiable function, in order to reduce the problem on a ball intersecting the boundary to a problem on the half-space

$$\mathbb{R}^d_+ \,=\, \big\{\xi\in\mathbb{R}^d \,\big|\, \xi=(\xi',\xi_d),\, \xi_d>0\big\}\,.$$

In contrast to [24, Section 4], we use general properties of Bernstein functions and of Modified Bessel functions of the Second Kind to compare $\mathrm{Tr}\big(\phi H^\Omega_{\mu,h}\phi\big)_-$ with[7] $\mathrm{Tr}\big(\phi H^+_{\mu,h}\phi\big)_-$ in Lemma 12 and Proposition 11.

By using the spectral representation of the generators of a class of stochastic processes on the half-line due to Kwaśnicki [37], we obtain an explicit diagonalization of $H^+_{\mu,h}$ in Sections 4 and 5. This is achieved by writing $A^+_{\mu/h}$ in terms of the family of one-dimensional model operators $\psi_{\mu/|\xi'|}(-\frac{d^2}{dt^2}{+}1)$, $\xi'\in\mathbb{R}^{d-1}$, with Dirichlet boundary condition on the half-line (see Lemma 14 and Proposition 15). By applying Kwaśnicki's results, we prove that the unitary operator $V_h : L^2(\mathbb{R}^d_+)\to L^2(\mathbb{R}^d_+)$ with integral kernel given by

$$v_h(\xi,x) := h^{-d/2}\, v(\xi,h^{-1}x)\,,\quad v(\xi,x) := |\xi'|^{1/2}\,\frac{e^{-i\xi' x'}}{(2\pi)^{(d-1)/2}}\sqrt{\frac{2}{\pi}}\, F_{\mu/|\xi'|,\xi_d}(|\xi'|x_d)\,, \tag{6.2}$$

establishes the unitary equivalence between $H^+_{\mu,h}$ and the operator of multiplication by the function $(\xi',\xi_d)\mapsto|\xi'|\psi_{\mu/|\xi'|}(\xi_d^2{+}1){-}1$. Note that, in contrast to the case of $\mu=0$ treated in [24], here the model operators and therefore the generalized eigenfunctions $F_{\mu/|\xi'|,\xi_d}$ depend on $\xi'\in\mathbb{R}^{d-1}$, which is due to the fact that ψ_μ is not homogeneous.

Similar to the analysis in the bulk (see (2.2) above), this diagonalization allows to compare $\mathrm{Tr}\big(\phi H^+_{\mu,h}\phi\big)_-$, for any $\phi\in C^1_0(\mathbb{R}^d)$, with its upper bound

$$\mathrm{Tr}\,\phi\big(H^+_{\mu,h}\big)_-\phi \,=\, \Lambda^{(1)}_\mu\, h^{-d}\int_{\mathbb{R}^d_+}\phi(x)^2dx - h^{-d+1}\int_{\mathbb{R}^d_+}\phi(x)^2h^{-1}\mathcal{K}_\mu(h^{-1}x_d)\,dx\,, \tag{6.5}$$

where

$$\mathcal{K}_\mu(t) = \frac{2}{(2\pi)^d}\int_{\mathbb{R}^{d-1}}|\xi'|^2\int_0^\infty\big(\psi_{\mu/|\xi'|}(\lambda^2{+}1)-|\xi'|^{-1}\big)_-\Big(1{-}2F_{\mu/|\xi'|,\lambda}(|\xi'|t)^2\Big)\,d\lambda\,d\xi'\,,$$

with an error term explicitly depending on μ and h (Lemmas 23 and 24). By using the technical Lemma 20, by which $\int_0^\infty t^\delta|\mathcal{K}_\mu(t)|\,dt \,\leqslant\, C_\delta\,(1{+}\mu)^{(d-\delta)/2}$ whenever $0\leqslant\delta<1$, this leads to appropriate upper and lower bounds on

$$\mathrm{Tr}\,\big(\phi H^+_{\mu,h}\phi\big)_- - h^{-d}\,\Lambda^{(1)}_\mu\int_{\mathbb{R}^d_+}\phi(x)^2dx + h^{-d+1}\Lambda^{(2)}_\mu\int_{\mathbb{R}^{d-1}}\phi(x',0)^2\,dx'\,,$$

where $\Lambda^{(2)}_\mu = \int_0^\infty\mathcal{K}_\mu(t)\,dt$ (see Proposition 21).

[7]Here $H^+_{\mu,h} := H^{\mathbb{R}^d_+}_{\mu,h}$, i.e. $H^+_{\mu,h} = hA^+_{\mu/h}-1$, where $A^+_{\mu/h} := A^{\mathbb{R}^d_+}_{\mu/h}$.

Finally, in Section 8, we complete the proof of Theorem 1 by combining the estimates from the analysis on the half-space, the straightening of the boundary, the bulk, and the localization, and choosing the localization parameter l_0 appropriately.

Conclusions

Riesz and Cesàro mean asymptotics. By substituting $h = \lambda^{-1}$, (0.16) is equivalent to the large-λ asymptotics of the Riesz mean

$$\sum_{n\in\mathbb{N}} \big(\lambda_n - \lambda\big)_- \;=\; \Lambda_0^{(1)}\,|\Omega|\,\lambda^{d+1} - \Big(\Lambda_0^{(2)}|\partial\Omega| - C_d\,|\Omega|\,m\Big)\,\lambda^d + \tilde{r}_m(\lambda)\,, \tag{0.17}$$

with $\tilde{r}_m(\lambda) = \lambda\, r_m(\lambda^{-1}) \in \mathcal{O}(\lambda^{d-\varepsilon})$ for any $\varepsilon \in (0, \gamma/(\gamma+2))$ when $\partial\Omega \in C^{1,\gamma}$ as $\lambda \to \infty$, and $\tilde{r}_m(\lambda) \in o(\lambda)$ when $\partial\Omega \in C^1$ as $\lambda \to \infty$. Hence, Theorem 2 is the direct generalization of the case $\alpha = 1$ in (0.8) for non-zero mass $m > 0$.

Moreover, as is shown in [24, Lemma A.1], from (0.16) we obtain for the N-th Cesàro mean of the eigenvalues of A_m^Ω,

$$\frac{1}{N}\sum_{n=1}^{N} \lambda_n \;=\; C_d^{(1)}|\Omega|^{-1/d}N^{1/d} + C_d^{(2)}\Big(\Lambda_0^{(2)}|\partial\Omega| - C_d\,|\Omega|\,m\Big)|\Omega|^{-1} + o(1) \quad \textit{as } N \to \infty\,, \tag{0.18}$$

where $C_d^{(1)} = \frac{(d+1)^{1+1/d}}{d}\big(\Lambda_0^{(1)}\big)^{-1/d}$ and $C_d^{(2)} = \frac{(d+1)^{2d+1}}{d^{2d}}\big(\Lambda_0^{(1)}\big)^{-1}$.

Heat trace asymptotics. In order to compare with the small-time asymptotics (0.7) of the heat trace $Z(t) = \sum_{n=1}^\infty e^{-\lambda_n t}$ for the eigenvalues of A_m^Ω, by Park and Song [45], note that the Laplace transform of the map $\lambda \to \sum_n (\lambda_n - \lambda)_-$ at $t > 0$ is given by $\frac{2}{t^2}Z(t)$. Hence, when $\partial\Omega \in C^{1,\gamma}$, we obtain from our result (0.17) that for all $\varepsilon \in (\gamma, (\gamma+2))$,

$$Z(t) = D^{(1)}|\Omega|\,t^{-d} - \big(D^{(2)}|\partial\Omega| - D^{(3)}|\Omega|\,m\big)\,t^{-d+1} + \mathcal{O}(t^{-d+1+\varepsilon})\,, \tag{0.19}$$

where $D^{(1)}$, $D^{(2)}$, and $D^{(3)}$ are the constants in (0.7) for $\alpha = 1$. For domains with $C^{1,\gamma}$ boundary, this is a slight improvement upon Park and Song's result, because their remainder is $o(t^{-d+1})$ for Lipschitz domains, and $\mathcal{O}(t^{-d+2})$ for domains with $C^{1,1}$ boundary.

Finitely many singularities. Since the contribution to (0.11) from a ball intersecting the boundary becomes arbitrarily small when $h \to 0$, it can be shown that our main result extends to Lipschitz domains with boundaries that are C^1 except at finitely many points.

More precisely, if $u_0 \in \partial\Omega$, then the support of the corresponding localization function ϕ_{u_0} is contained in a ball with radius $l(u_0) \leqslant \frac{l_0}{2}$, where the localization parameter l_0 becomes arbitrarily small when $h \to 0$ (see Sections 1 and 8). Therefore, it can be shown that the contribution from a finite number of points $u_j \in \partial\Omega$, $j = 1, \dots, N$, is negligible in the limit $h \to 0$, under the condition that there exist positive constants R and C, only depending on the dimension d and Ω, such that

$$\big|\partial\Omega \cap B_r(u_j)\big| \;\leqslant\; C\,r^{d-1} \qquad \forall j = 1, \dots, N$$

for all $r \leqslant R$. For instance, this condition is satisfied in $d = 2$ by any simple polygon.

Non-relativistic limit. Since, for $c \to \infty$, the operator $A_c^\Omega = (\sqrt{-c^2\Delta+c^4}-c^2)_D$ converges in resolvent sense to $\frac{1}{2}(-\Delta)_D$, and in particular its eigenvalues $\lambda_n(c)$ converge (pointwise) to those of $\frac{1}{2}(-\Delta)_D$, it would be interesting if we were able to recover the asymptotic formula [22] for the N-th Cesàro mean of the eigenvalues of $\frac{1}{2}(-\Delta)_D$ as $N \to \infty$ from our result for A_c^Ω by passing to the limit $c \to \infty$. For that purpose, similarly as for small μ (Appendix F.1), it can be shown that for all $\mu > 0$

$$\Big|\mu^{-d/2}\Lambda_\mu^{(1)} - L_d\Big| \leqslant c\,\mu^{-1}, \quad \Big|\mu^{-(d-1)/2}\Lambda_\mu^{(2)} - \frac{L_{d-1}}{4}\Big| \leqslant c\,\mu^{-1/2},$$

where $L_d := (2\pi)^{-d}\int(p^2-1)_-\,dp$ and $\frac{L_{d-1}}{4}$ are the corresponding constants for $(-\Delta)_D$ in [22]. By applying Theorem 1 with $\mu = c^2/\lambda$ and $h = c/\lambda$, for fixed λ, the first two terms in the resulting formula for $\sum_n(\lambda_n(c)-\lambda)_-$, are independent of c and coincide with the first two terms in [22], while the remainder converges to zero as $c \to \infty$, expressing the fact that the spectrum of $(\sqrt{-c^2\Delta+c^4}-c^2)_D$ converges pointwise to the spectrum of $\frac{1}{2}(-\Delta)_D$ as $c \to \infty$. However, due to the factor $(1+\mu)^{d/2}$ in the remainder in (0.11), even if we let c depend on λ, the second term in (0.11) always has the same or a higher order of λ as the remainder, and so [22] can not be re-obtained from our result.

Other powers $\alpha \in (0,2)$. Regarding the results of Frank and Geisinger [24] and the results of Park and Song [45], it is reasonable to ask whether the approach used in this thesis can be applied to the operator

$$((-\Delta+m^{2/\alpha})^{\alpha/2}-m)_D \tag{0.20}$$

with Dirichlet boundary condition on Ω, for arbitrary $\alpha \in (0,2)$. The work [37] by Kwaśnicki, i.e. the explicit diagonalization of the generators of certain Lévy processes on the half-line, which our method is based on, is also applicable for (0.20). In fact, Kwaśnicki's diagonalization works for Lévy processes with Lévy exponent of the form $f(\xi^2)$, where f is a Bernstein function satisfying $f(0) = 0$, and the function $f_{\omega,\alpha} : \mathbb{R}_+ \to \mathbb{R}_+$, given by

$$f_{\omega,\alpha}(t) := (t+1+\omega^{2/\alpha})^{\alpha/2} - (1+\omega^{2/\alpha})^{\alpha/2},$$

is such a Bernstein function for any $\omega > 0$ and $\alpha \in (0,2)$ (see (5.10) and Section E.7). However, our proof of Proposition 11 (straightening of the boundary) relies on an integral representation of Modified Bessel functions of the Second Kind (identity (D.7)), which loses the properties we are making use of, whenever $\alpha < 1$. Other than that, besides a technically more sophisticated analysis of the generalized eigenfunctions of the model operators, there is no reason why the method is not applicable in that case, and of course, it might be possible to prove Proposition 11 by other means.

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List of symbols

A_m^Ω	$(\sqrt{-\Delta+m^2}-m)_D$ with Dirichlet boundary condition on $\Omega\subset\mathbb{R}^d$, see (0.1)
A_m^+	A_m^Ω with $\Omega=\mathbb{R}^d_+$, see Section 3
$B_r(y)$	$\{x\in\mathbb{R}^d \,\|\, \|x-y\|<r\}$, open ball in $\mathbb{R}^d$ with center $y\in\mathbb{R}^d$ and radius $r>0$
C	Constants[8] independent of the parameters h, μ, and l_0
$C_0^k(X)$	k-times continuously differentiable functions on X with compact support
$\mathcal{F}^{(d-1)}$	Partial Fourier transform in $L^2(\mathbb{R}^d)$ w.r.t. the first $d-1$ variables, see (4.1)
$F_{\omega,\lambda}$	Generalized eigenfunctions of $(\sqrt{d^2/dt^2+1+\omega^2}-\sqrt{1+\omega^2})_D$, see Corollary 17
$G_{\omega,\lambda}$	Second term in $F_{\omega,\lambda}$, see (5.3)
$H^s(\Omega)$	Fractional Sobolev space of order $s\in(0,1)$, see Appendix A
$H_{\mu,h}^\Omega$	$hA_{\mu/h}^\Omega-1$ for $h,\mu>0$
$H_{\mu,h}$	$H_{\mu/h}^\Omega$ with $\Omega=\mathbb{R}^d$, see Section 2
$H_{\mu/h}^+$	$H_{\mu/h}^\Omega$ with $\Omega=\mathbb{R}^d_+$, see Section 3
$\mathcal{K}_\mu$	Integrand in $\Lambda_\mu^{(2)}=\int_0^\infty\mathcal{K}_\mu(t)\,dt$, see (5.23)
K_β	Modified Bessel function of the Second Kind of order $\beta\in\mathbb{R}$, see Appendix D.2
l_0	Localization parameter, see definition of $l(u)$ in (1.1)
$l(u)$	Radii of the balls containing the supports of the functions ϕ_u, see (1.1)
$\Lambda_\mu^{(1)}$	$(2\pi)^{-d}\int_{\mathbb{R}^d}(\psi_\mu(\|\xi\|^2)-1)_- d\xi$, see (0.12)
$\Lambda_\mu^{(2)}$	Second constant in Theorem 1, see also (5.21)
$a\wedge b$	$\min\{a,b\}$ for $a,b\in\mathbb{R}$
$(t)_-$	$\frac{1}{2}(\|t\|-t)=-(t\wedge 0)$ for $t\in\mathbb{R}$
ϕ_u	Localization function at $u\in\mathbb{R}^d$, see (1.3)
$\psi_m(t)$	$\sqrt{t+m^2}-m$, see (0.9)
q_A	Quadratic form of a self-adjoint operator A
q_m^Ω	Quadratic form of A_m^Ω, see (0.1)
$\mathbb{R}^d_+$	Half-space $\{\xi\in\mathbb{R}^d \,\|\, \xi=(\xi',\xi_d),\xi_d>0\}$
$\mathbb{S}^d$	$\{x\in\mathbb{R}^{d+1} \,\|\, \|x\|=1\}$, d-dimensional unit sphere
$\theta(t)$	Integration factor in the representation (0.10) of q_m^Ω, see proof of Lemma 6
$\vartheta_\omega(\lambda)$	Phaseshift in the expression (5.3) of $F_{\omega,\lambda}$, see (5.9)
$v_h(\xi,x)$	Integral kernel of the unitary operator V_h diagonalizing $hA_{\mu/h}^+$, see Lemma 22
$w(t)$	Modulus of continuity of Ω, see Section 3

[8]Constants denoted by the letter C may have different values even if they occur several times in a series of equations or inequalities.

1. Localization

Following [50] and [24], for $l_0 \in \mathbb{R}$ with $0 < l_0 < \frac{1}{2}$ let $l : \mathbb{R}^d \to [0, \infty)$ be given by

$$l(u) = \frac{1}{2}\Big(1 + \big(\delta(u)^2 + l_0^2\big)^{-1/2}\Big)^{-1}, \tag{1.1}$$

where $\delta(u) := \operatorname{dist}(u, \Omega^c) = \inf\{|x-u| : x \in \Omega^c\}$ denotes the distance of $u \in \mathbb{R}^d$ to the complement $\Omega^c = \mathbb{R}^d \backslash \Omega$. The following lemma provides basic properties of $l(u)$, which will be important in the following.

Lemma 3. *The function l defined in* (1.1) *satisfies $\frac{l_0}{3} < l(u) < \frac{1}{2}$. Moreover, l has partial derivatives almost everywhere on $\mathbb{R}^d$, and $\|\nabla l\|_\infty \leqslant \frac{1}{2}$.*

Proof. First, $\frac{l_0}{3} < l(u) < \frac{1}{2}$ immediately follows from $0 < l_0 < \frac{1}{2}$. Next, since the distance function δ is Lipschitz continuous, by Rademacher's theorem (see for instance [18, Sect. 3.1]) it is almost everywhere differentiable. Moreover, by [17, Theorem 5.1.5], δ is differentiable in $x \in \Omega$ iff x has a unique nearest point $y \in \Omega^c$, and in this case $\nabla\delta(x) = \frac{y-x}{|y-x|}$. Hence, for a.e. $x \in \Omega$ there exists $y \in \Omega^c$ such that $|\nabla l(x)| \leqslant \frac{1}{2}|\frac{y-x}{|y-x|}| = \frac{1}{2}$. □

For each $x \in \mathbb{R}^d$ let J_x denote the Jacobian of the map $u \mapsto l(u)^{-1}(x-u)$, i.e.

$$J_x(u) = l(u)^{-d} \left|\det\left(\frac{x_i - u_i}{l(u)}\partial_j l(u) + \delta_{ij}\right)_{ij}\right| \qquad \text{for a.e. } u \in \mathbb{R}^d, \tag{1.2}$$

let $\phi \in C_0^\infty(\mathbb{R}^d)$ be real-valued with $\operatorname{supp}\phi \subset B_1(0) = \{x \in \mathbb{R}^d \,|\, |x| < 1\}$ and $\|\phi\|_2 = 1$, and for a.e. $u \in \mathbb{R}^d$, let $\phi_u \in C_0^\infty(\mathbb{R}^d)$ be given by

$$\phi_u(x) := l(u)^{d/2}\sqrt{J_x(u)}\;\phi\left(\frac{x-u}{l(u)}\right). \tag{1.3}$$

Lemma 4. *For a.e. $u \in \mathbb{R}^d$ we have $\operatorname{supp}\phi_u \subset B_{l(u)}(u)$, $\|\phi_u\|_\infty \leqslant C$, $\|\nabla\phi_u\|_\infty \leqslant C\,l(u)^{-1}$, where both constants can be chosen independently of u and l_0. Moreover, for all $x \in \mathbb{R}^d$,*

$$\int_{\mathbb{R}^d} \phi_u(x)^2\, l(u)^{-d} du = 1. \tag{1.4}$$

Proof. The first three properties are immediate consequences of $\operatorname{supp}\phi \subset B_1(0)$ and of Definition (1.3). For (1.4), let J_x^l denote the Jacobian (1.2) and let $l_x(u) := l(u+x)$, so that $J_x^l(u+x) = J_0^{l_x}(u)$ for a.e. $u \in \mathbb{R}^d$. Hence, it suffices to prove that $\int_{\mathbb{R}^d} \phi(F(u))^2 J_0^{l_x}(u)\,du = 1$, where for fixed $x \in \mathbb{R}^d$ we write $F(u) := -l_x(u)^{-1}u$. It follows that F is injective on $F^{-1}(B_1(0))$, since we have $F(u) = F(v)$ if and only if $v = tu$ for some $t \in \mathbb{R}$. Moreover, $F(tu) = -g(t)u$ with $g : \mathbb{R} \to \mathbb{R}$ monotonically increasing in t for all $t \in \mathbb{R}$ and for all u for which $|g(t)||u| \leqslant 1$. In fact, $g(t) = t/l_x(tu)$ for all $t \in \mathbb{R}$, and thus

$$g'(t) = l_x(tu)^{-1} - t l_x(tu)^{-2}\nabla l_x(tu)\cdot u \geqslant l_x(tu)^{-1}\big(1 - \|\nabla l_x\|_\infty |g(t)||u|\big) > 0,$$

since $\|\nabla l_x\|_\infty \leqslant \frac{1}{2}$ and $|g(t)||u| \leqslant 1$.

By the change of variables formula for Lipschitz functions (see for instance [29, Thm. 2]) it follows that $\int_{\mathbb{R}^d} \phi(F(u))^2 J_0^{l_x}(u)\,du = \|\phi\|_2^2 = 1$, since $\operatorname{supp}(\phi\circ F) \subset F^{-1}(B_1(0))$. □

Note that, due to (1.4), the family $\{\phi_u\}_{u\in\mathbb{R}^d}$ can be viewed as a partition of unity with respect to the continuous parameter u. In fact, equation (1.4) gives rise to an IMS-type localization formula (see Lemma 6 below), which will be the key ingredient in the proof of the following proposition, the main result of this section.

Proposition 5. *There exists $C>0$ such that for all $\mu>0$, $0<l_0<\frac{1}{2}$, and $0<h\leqslant\frac{l_0}{8}$*

$$0 \;\leqslant\; \operatorname{Tr}\big(H^{\Omega}_{\mu,h}\big)_- - \int_{\mathbb{R}^d} \operatorname{Tr}\big(\phi_u H^{\Omega}_{\mu,h}\phi_u\big)_-\, l(u)^{-d}\,du \;\leqslant\; C\,h^{-d+2}\,l_0^{-1}\,\mathfrak{S}_d(l_0/h)\,(1+\mu)^{d/2}\,, \tag{1.5}$$

where

$$\mathfrak{S}_d(t) \;:=\; \begin{cases} 1\,, & d>2 \\ |\ln(t)|^{1/2}\,, & d=2\,. \end{cases}$$

The proof is based on methods from [40]. First, in Lemma 6, we will establish a localization formula similar to [40, Theorem 9], which allows to express $\operatorname{Tr}\rho A^{\Omega}_m$, for a suitable trace class operator ρ, in terms of the localized versions $\operatorname{Tr}\rho\phi_u A^{\Omega}_m\phi_u$. This is done at the expense of an error that involves terms of the form $\operatorname{Tr}\rho L_u$, where, for $u\in\mathbb{R}^d$, L_u is the bounded integral operator with kernel given by (1.6) below. This error will be controlled by estimate (1.8). The corresponding results in the case $d=3$ have been shown in [50, Theorems 2.5, 2.6].

Lemma 6 (Localization formula). *Let Ω^* be the set of all $u\in\mathbb{R}^d$ with $\operatorname{supp}\phi_u\cap\Omega\neq\emptyset$. Then, for all $u\in\mathbb{R}^d$, the integral operator L_u in $L^2(\mathbb{R}^d)$ with kernel*

$$L_u(x,y) := \Big(\frac{\mu}{2\pi h}\Big)^{(d+1)/2} |\phi_u(x)-\phi_u(y)|^2\,\frac{K_{(d+1)/2}(\mu|x-y|/h)}{|x-y|^{(d+1)/2}}\,\chi_\Omega(x)\chi_\Omega(y) \tag{1.6}$$

is bounded, $\|L_u\|\leqslant C\,\mu^{-1}h\,l(u)^{-2}$, and for all $f\in H^{1/2}_0(\Omega)$,

$$q^{\Omega}_{\mu/h}(f) = \int_{\Omega^*} q^{\Omega}_{\mu/h}(f\phi_u)\,l(u)^{-d}\,du - \int_{\Omega^*}(f,L_uf)\,l(u)^{-d}\,du\,. \tag{1.7}$$

Proof. If, for $t,\nu>0$, we define $\theta(t):=(2\pi t)^{-(d+1)/2}\,K_{(d+1)/2}(t)$ and $\theta_\nu(t):=\nu^{d+1}\theta(\nu t)$, then by (0.10), for all $f\in H^{1/2}_0(\Omega)$,

$$\begin{aligned} q^{\Omega}_{\mu/h}(f) \;&=\; \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} |f(x)-f(y)|^2\,\theta_{\mu/h}(|x-y|)\,dx\,dy \\ &=\; \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \Big(|f(x)|^2+|f(y)|^2-\overline{f(x)}\,f(y)-f(x)\,\overline{f(y)}\Big)\,\theta_{\mu/h}(|x-y|)\,dx\,dy \\ &\overset{(1.4)}{=}\; \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \Big(|f(x)|^2\phi_u(x)^2+|f(y)|^2\phi_u(y)^2\Big)\,\theta_{\mu/h}(|x-y|)\,\frac{du}{l(u)^d}\,dx\,dy \\ &\qquad -\frac{1}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\Big(\phi_u(x)^2+\phi_u(y)^2\Big)\Big(\overline{f(x)}f(y)+f(x)\overline{f(y)}\Big)\theta_{\mu/h}(|x-y|)\,\frac{du}{l(u)^d}\,dx\,dy \\ &=\; \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\Omega^*} |f\phi_u(x)-f\phi_u(y)|^2\,\theta_{\mu/h}(|x-y|)\frac{du}{l(u)^d}\,dx\,dy - \int_{\Omega^*}(f,L_uf)\,\frac{du}{l(u)^d}\,. \end{aligned}$$

In the last step, we have inserted $0=\phi_u(x)\phi_u(y)-\phi_u(x)\phi_u(y)$ in the second integrand, and we have used that $f(x)\phi_u(x)=0$ whenever $u\in\mathbb{R}^d\setminus\Omega^*$. Since the function $(x,y,u)\mapsto(\phi_u(x)-\phi_u(y))^2\,\overline{f(x)}\,f(y)\,\theta_{\mu/h}(|x-y|)\,l(u)^{-d}$ is absolutely integrable, equation (1.7) follows by using Fubini's theorem.

Next, for the boundedness of L_u, note that, due to $K_{(d+1)/2}(t) \leqslant C\, t^{-(d+1)/2} e^{-t/2}$ (see Lemma 31 in Appendix D.2), we have $\int_0^\infty K_{(d+1)/2}(t)\, t^{(d+1)/2}\, dt < \infty$. For any $f \in L^2(\mathbb{R}^d)$,

$$
\begin{aligned}
|(f, L_u f)| \;&\leqslant\; \Big(\frac{\mu}{2\pi h}\Big)^{(d+1)/2} \|\nabla\phi_u\|_\infty^2 \int_{\mathbb{R}^d} |f(x)| \int_{\mathbb{R}^d} \frac{K_{(d+1)/2}(\mu\,|x-y|/h)}{|x-y|^{(d-3)/2}}\, |f(y)|\, dx\, dy \\
&\leqslant\; C\, l(u)^{-2} \Big(\frac{\mu}{h}\Big)^{(d+1)/2} \|f\|_2 \, \Big\| \frac{K_{(d+1)/2}(\mu\,|\cdot|/h)}{|\cdot|^{(d-3)/2}} * |f| \Big\|_2 .
\end{aligned}
$$

Since by Young's inequality, $\|g * h\|_2 \leqslant \|g\|_1 \|h\|_2$, whenever $g \in L^1(\mathbb{R}^d)$ and $h \in L^2(\mathbb{R}^d)$, it follows that L_u is bounded. Moreover,

$$
\Big(\frac{\mu}{h}\Big)^{(d+3)/2} \Big\| \frac{K_{(d+1)/2}(\mu\,|\cdot|/h)}{|\cdot|^{(d-3)/2}} \Big\|_1 \;=\; |\mathbb{S}^{d-1}| \int_0^\infty K_{(d+1)/2}(t)\, t^{(d+1)/2}\, dt \;=\; C\,,
$$

and therefore $\|L_u\| \leqslant C\, \mu^{-1} h\, l(u)^{-2}$. □

The following result will be used to control the second term in (1.7).

Lemma 7 (**Localization error**). *There exists $C > 0$ such that for all $u \in \mathbb{R}^d$, $0 < \delta \leqslant \frac{1}{2}$, and all positive definite trace class operators ρ,*

$$
\operatorname{Tr} \rho L_u \;\leqslant\; C\, l(u)^{-1} \Big(\delta\, \operatorname{Tr}(\rho\, \chi_\Omega\, \chi_{u,\delta}) + \tau_d(\delta)\, \|\rho\| \Big)\,, \tag{1.8}
$$

where $\chi_{u,\delta}$ denotes the characteristic function of the ball $B_{l(u)(1+\delta)}(u)$, and

$$
\tau_d(\delta) \;:=\; \begin{cases} \delta^{-d+2}\,, & d > 2 \\ |\ln(\delta)|\,, & d = 2\,. \end{cases} \tag{1.9}
$$

Proof. We first prove the statement for

$$
L^\Lambda(x,y) := \Big(\frac{\mu}{2\pi h}\Big)^{(d+1)/2} |\phi_0(x) - \phi_0(y)|^2 \, \frac{K_{(d+1)/2}(\mu|x-y|/h)}{|x-y|^{(d+1)/2}}\, \chi_\Lambda(x,y)\,,
$$

where $\Lambda \subset \mathbb{R}^d \times \mathbb{R}^d$ denotes a given bounded set, in particular $L^{\Omega\times\Omega} = L_0$.

We split L^Λ into a short and a long range part, L_s^Λ and L_l^Λ respectively, by setting

$$
L_s^\Lambda(x,y) := \begin{cases} (\chi_{0,\delta}\, L^\Lambda\, \chi_{0,\delta})(x,y) & \text{if } |x-y| < l(0)\,\delta \\ 0 & \text{if } |x-y| \geqslant l(0)\,\delta \end{cases}\,,
$$

and $L_l^\Lambda(x,y) := L^\Lambda(x,y) - L_s^\Lambda(x,y)$. As a first step, by an adaption of the arguments used in [40] to arrive at [40, eq. (6.8)], we show for any $\varepsilon > 0$ that

$$
\operatorname{Tr} \rho L^\Lambda \;\leqslant\; \operatorname{Tr} \rho(\iota + \varepsilon\chi) + \frac{\|\rho\|}{2\varepsilon} \operatorname{Tr}\big[(L_l^\Lambda)^2\big], \tag{1.10}
$$

where $\chi := \chi_{B_{l(0)}(0)}$ denotes the characteristic function of the ball $B_{l(0)}(0)$, $\|\rho\|$ denotes the operator norm of ρ, and $\iota(x) := \int L_s^\Lambda(x,y)\, dy$.

Since $\rho^{1/2}$ and $\rho^{1/2}L_l^\Lambda$ are Hilbert-Schmidt operators, it follows from the cyclicity of the trace, and from $L^\Lambda(x,y) = L^\Lambda(y,x)$ that

$$\begin{aligned}\operatorname{Tr}\rho L_l^\Lambda \;&=\; \operatorname{Tr}\rho^{1/2}L_l^\Lambda\rho^{1/2} \;=\; \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\rho^{1/2}(z,x)\,L_l^\Lambda(x,y)\,\rho^{1/2}(y,z)\,dx\,dy\,dz\\ &=\; 2\ \mathrm{Re}\left(\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{|x|>|y|}\rho^{1/2}(z,x)\,L_l^\Lambda(x,y)\,\rho^{1/2}(y,z)\,dx\,dy\,dz\right).\end{aligned}$$

If $|x|,|y| > l(0)$ then $L^\Lambda(x,y) = 0$, since $\operatorname{supp}\phi_0 \subset B_{l(0)}(0)$. Hence, from $2ab \leqslant \varepsilon a^2 + \varepsilon^{-1}b^2$ for all $a, b \in \mathbb{R}$ and $\varepsilon > 0$, it follows that

$$\begin{aligned}\operatorname{Tr}\rho L_l^\Lambda \;&=\; 2\ \mathrm{Re}\left(\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\chi(y)\,\rho^{1/2}(y,z)\left(\int_{|x|>|y|}\rho^{1/2}(z,x)\,L_l^\Lambda(x,y)\,dx\right)dy\,dz\right)\\ &\leqslant\; \varepsilon\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\chi(y)\,|\rho^{1/2}(y,z)|^2\,dy\,dz + \varepsilon^{-1}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\chi(y)\,\omega(y,z)\,dy\,dz\,, \qquad (1.11)\end{aligned}$$

where we have set

$$\begin{aligned}\omega(y,z) \;&:=\; \left|\int_{|x|>|y|}\rho^{1/2}(z,x)L_l^\Lambda(x,y)\,dx\right|^2\\ &=\; \int_{|\xi|>|y|}\int_{|x|>|y|}\overline{\rho^{1/2}(z,\xi)}\,\rho^{1/2}(z,x)\,L_l^\Lambda(\xi,y)\,L_l^\Lambda(x,y)\,dx\,d\xi\,.\end{aligned}$$

First, for the second term in (1.11), by the Cauchy-Schwarz inequality we have

$$\begin{aligned}&\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}|\rho^{1/2}(z,\xi)|\,|\rho^{1/2}(z,x)|\,L_l^\Lambda(\xi,y)\,L_l^\Lambda(x,y)\,dz\,d\xi\,dx\,dy\\ &\leqslant\; \int_{\mathbb{R}^d}\left(\int_{\mathbb{R}^d}\left\|\rho^{1/2}(\cdot,\xi)\right\|_2 L_l^\Lambda(\xi,y)\,d\xi\right)^2 dy \;\leqslant\; \left\|\rho^{1/2}\right\|_2^2\left\|L_l^\Lambda\right\|_2^2 \;<\; \infty\,.\end{aligned}$$

Therefore, by Fubini's theorem

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\chi(y)\,\omega(y,z)\,dy\,dz \;=\; \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\rho^{1/2}(z,x)\,A(x,\xi)\,\rho^{1/2}(\xi,z)\,dx\,d\xi\,dz \;=\; \operatorname{Tr}\rho A\,,$$

where A denotes the Hilbert-Schmidt operator with integral kernel given by

$$A(x,\xi) \;:=\; \int_{|y|<\min\{|x|,|\xi|\}}\chi(y)\,L_l^\Lambda(x,y)\,L_l^\Lambda(\xi,y)\,dy\,,$$

and we have used that $\operatorname{Tr}AB = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}A(y,x)B(x,y)\,dx\,dy$ if A and B are Hilbert-Schmidt operators in $L^2(\mathbb{R}^d)$ [26, Lemma VI.7.16]. Since $A, \rho \geqslant 0$, we have

$$\begin{aligned}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\chi(y)\,\omega(y,z)\,dy\,dz \;&=\; \operatorname{Tr}\rho A \;=\; \|\rho A\|_1 \;\leqslant\; \|\rho\|\,\|A\|_1\\ &=\; \|\rho\|\int_{\mathbb{R}^d}\int_{|x|>|y|}L_l^\Lambda(x,y)^2\,dx\,dy \;=\; \frac{\|\rho\|}{2}\operatorname{Tr}\left[(L_l^\Lambda)^2\right], \qquad (1.12)\end{aligned}$$

where $\|A\|_1$ denotes the trace norm of a trace class operator ρ. Since

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\chi(y)|\rho^{1/2}(y,z)|^2\,dy\,dz \;=\; \operatorname{Tr}\rho^{1/2}\chi\rho^{1/2} \;=\; \operatorname{Tr}\chi\rho\,,$$

it follows from (1.11) and (1.12) that

$$\operatorname{Tr}\rho L_l^\Lambda \;\leqslant\; \varepsilon\operatorname{Tr}\rho\chi + \frac{\|\rho\|}{2\varepsilon}\operatorname{Tr}\left[(L_l^\Lambda)^2\right]. \qquad (1.13)$$

If $\{\psi_j\}_{j\in I} \subset L^2(\mathbb{R}^d)$ and $\{\mu_j\}_{j\in I} \subset \mathbb{R}_+$ are such that $\rho = \sum_{j\in I} \mu_j(\psi_j,\cdot)\psi_j$ is the singular value decomposition of ρ, then

$$\begin{aligned}
\operatorname{Tr}\rho L_s^\Lambda &= \sum_{j\in I} \mu_j\,(\psi_j, L_s^\Lambda \psi_j) \leqslant \sum_{j\in I} \mu_j \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} L_s^\Lambda(x,y)\,|\psi_j(x)|\,|\psi_j(y)|\,dx\,dy \\
&\leqslant \sum_{j\in I} \mu_j \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} L_s^\Lambda(x,y)\,\tfrac{1}{2}\Big(|\psi_j(x)|^2 + |\psi_j(y)|^2\Big)\,dx\,dy \\
&= \sum_{j\in I} \mu_j \int_{\mathbb{R}^d} \iota(x)\,|\psi_j(x)|^2\,dx \;=\; \operatorname{Tr}\rho\,\iota\,,
\end{aligned}$$

since $\iota(x) = \int L_s^\Lambda(x,y)\,dy$. Together with (1.13), this concludes the proof of (1.10).

We continue with bounds for ι and $\operatorname{Tr}\big[(L_l^\Lambda)^2\big]$. By definition, for any $x \in \mathbb{R}^d$,

$$\begin{aligned}
\iota(x) &= \chi_{0,\delta}(x) \int_{|x-y|<l(0)\,\delta} L^\Lambda(x,y)\,\chi_{0,\delta}(y)\,dy \\
&\leqslant \chi_{0,\delta}(x)\,\|\nabla\phi_0\|_\infty^2 \left(\frac{\mu}{2\pi h}\right)^{(d+1)/2} \int_{|x-y|<l(0)\delta} \frac{K_{(d+1)/2}(\mu|x-y|/h)}{|x-y|^{(d-3)/2}}\,dy \\
&\leqslant C\,\chi_{0,\delta}(x)\,l(0)^{-2}\mu^{-1}h \int_0^{l(0)\,\delta\,\mu/h} K_{(d+1)/2}(t)\,t^{(d+1)/2}\,dt \\
&\leqslant C\,\chi_{0,\delta}(x)\,l(0)^{-2}\mu^{-1}h\,\Big(1 - e^{-l(0)\,\delta\,\mu/(2h)}\Big) \\
&\leqslant C\,\chi_{0,\delta}(x)\,l(0)^{-1}\delta\,\min\big\{1, l(0)^{-1}\delta^{-1}\mu^{-1}h\big\}\,. \qquad (1.14)
\end{aligned}$$

Next, assuming $L^\Lambda(x,y) \neq 0$ and $|x|>|y|$, then $|y| \leqslant l(0)$. If additionally $|x-y| < l(0)\,\delta$, then $|x| \leqslant |x-y| + |y| < l(0)(1+\delta)$, and therefore $\chi_{0,\delta}L^\Lambda\chi_{0,\delta}(x,y) = L^\Lambda(x,y)$, i.e. $L_l^\Lambda(x,y) = 0$. Thus, if

$$D_\delta := \big\{(x,y) \in \mathbb{R}^d \times \mathbb{R}^d \,\big|\, |x|>|y|, |y| \leqslant l(0), |x-y| \geqslant l(0)\,\delta\big\}\,,$$

then

$$\begin{aligned}
\operatorname{Tr}\big[(L_l^\Lambda)^2\big] &= 2\int\int_{|x|>|y|} L_l^\Lambda(x,y)^2\,dx\,dy \\
&= C\,(\mu/h)^{d+1} \int\int_{D_\delta} \left(|\phi_0(x)-\phi_0(y)|^2 \frac{K_{(d+1)/2}(\mu|x-y|/h)}{|x-y|^{(d+1)/2}}\right)^2 dx\,dy \\
&= C\,(\mu/h)^{d+1} \Bigg(\int\int_{D_\delta\cap\{|x|\geqslant 2l(0)\}} |\phi_0(x)-\phi_0(y)|^4\,\frac{K_{(d+1)/2}(\mu|x-y|/h)^2}{|x-y|^{d+1}}\,dx\,dy \\
&\qquad + \int\int_{D_\delta\cap\{|x|<2l(0)\}} |\phi_0(x)-\phi_0(y)|^4\,\frac{K_{(d+1)/2}(\mu|x-y|/h)^2}{|x-y|^{d+1}}\,dx\,dy \Bigg)\,.
\end{aligned}$$

Since $\phi_0(x)=0$ whenever $|x|>l(0)$, it follows that

$$\begin{aligned}
\operatorname{Tr}\left[(L_l^\Lambda)^2\right] \;&\leqslant\; C\,\mu^{d+1}h^{-d-1}\Bigg(\int\!\!\int_{D_\delta\cap\{|x|\geqslant 2l(0)\}}\phi_0(y)^4\,\frac{K_{(d+1)/2}(\mu|x-y|/h)^2}{|x-y|^{d+1}}\,dx\,dy \\
&\qquad + \;\|\nabla\phi_0\|_\infty^4\int\!\!\int_{D_\delta\cap\{|x|<2l(0)\}}\frac{K_{(d+1)/2}(\mu|x-y|/h)^2}{|x-y|^{d-3}}\,dx\,dy\Bigg) \\
&=:\; C\,\mu^{d+1}h^{-d-1}\Big(I_\delta+\|\nabla\phi_0\|_\infty^4\,J_\delta\Big)\,. \qquad (1.15)
\end{aligned}$$

Since, for $(x,y)\in D_\delta\cap\{|x|\geqslant 2l(0)\}$, we have $|x-y|\geqslant|x|-|y|\geqslant l(0)$, we obtain

$$\begin{aligned}
I_\delta \;&\leqslant\; C\,|B_{l(0)}(0)|\int_{|z|\geqslant l(0)}K_{(d+1)/2}(\mu|z|/h)^2\,|z|^{-d-1}\,dz \\
&=\; C\,l(0)^d\mu\,h^{-1}\int_{l(0)\,\mu/h}^{\infty}K_{(d+1)/2}(t)^2\,t^{-2}\,dt \\
&\leqslant\; C\,l(0)^d\mu\,h^{-1}\int_{l(0)\,\mu/h}^{\infty}t^{-d-3}\,e^{-t}dt \\
&=\; C\,l(0)^{-2}\mu^{-d-1}h^{d+1}\,.
\end{aligned}$$

Next, for $(x,y)\in D_\delta\cap\{|x|<2l(0)\}$ we have $|x-y|\leqslant|x|+|y|\leqslant 3l(0)$, and therefore

$$\begin{aligned}
J_\delta \;&\leqslant\; |B_{l(0)}(0)|\int_{l(0)\delta\leqslant|z|\leqslant 3l(0)}K_{(d+1)/2}(\mu|z|/h)^2\,|z|^{-d+3}\,dz \\
&=\; C\,l(0)^d\mu^{-3}h^3\int_{l(0)\delta\mu/h}^{3l(0)\mu/h}K_{(d+1)/2}(t)^2\,t^2\,dt \\
&\leqslant\; C\,l(0)^d\mu^{-3}h^3\int_{l(0)\delta\mu/h}^{3l(0)\mu/h}t^{-d+1}\,e^{-t}\,dt \\
&\leqslant\; C\,l(0)^2\mu^{-d-1}h^{d+1}\int_\delta^3 s^{-d+1}e^{-l(0)\mu s/h}\,ds \\
&\leqslant\; C\,l(0)^2\mu^{-d-1}h^{d+1}\begin{cases}\delta^{-d+2}\,, & d>2\\ |\ln(\delta)|\,, & d=2\,.\end{cases}\;,
\end{aligned}$$

Since $\|\nabla\phi_0\|_\infty\leqslant C\,l(0)^{-1}$ and $\delta\leqslant 1/2$, by using the upper bounds on I_δ and J_δ in (1.15), we obtain

$$\operatorname{Tr}[(L_l^\Lambda)^2]\leqslant C\,l(0)^{-2}\,\tau_d(\delta)$$

with $\tau_d(\delta)$ as defined in (1.9). Together with (1.14), inserted in (1.10), this implies

$$\operatorname{Tr}\rho L^\Lambda \;\leqslant\; C\,l(0)^{-1}\delta\operatorname{Tr}\rho\chi_{0,\delta}+\varepsilon\operatorname{Tr}\rho\chi+C\,\frac{\|\rho\|}{2\varepsilon}\,l(0)^{-2}\,\tau_d(\delta)\,.$$

Putting $\varepsilon=l(0)^{-1}\delta$ and noting that $\chi=\chi_{0,0}\leqslant\chi_{0,\delta}$, we obtain

$$\operatorname{Tr}\rho L^\Lambda \;\leqslant\; C\,l(0)^{-1}\Big(\delta\operatorname{Tr}(\rho\chi_{0,\delta})+\tau_d(\delta)\,\|\rho\|\Big)\,. \qquad (1.16)$$

In order to obtain (1.8), we observe that replacing ϕ_0 by the shifted version of ϕ_u with support in the ball $B_{l(u)}(0)$ centered at 0, namely $\tilde\phi_u:=\phi_u(\cdot+u)$, besides of the replacement of $l(0)$ by $l(u)$, does not change any of the estimates in the calculations above. So, if $\tilde{L}_u^\Lambda$ denotes the corresponding modification of L^Λ where ϕ_0 is replaced by $\tilde{\phi}_u$, i.e.

$$\tilde{L}^\Lambda(x,y) := \Big(\frac{\mu}{2\pi h}\Big)^{(d+1)/2} |\tilde{\phi}_u(x)-\tilde{\phi}_u(y)|^2 \, \frac{K_{(d+1)/2}(\mu|x-y|/h)}{|x-y|^{(d+1)/2}} \, \chi_\Lambda(x,y)\,,$$

then, by (1.16),

$$\operatorname{Tr}\rho\tilde{L}_u^\Lambda \;\leqslant\; C\,l(u)^{-1}\Big(\delta\operatorname{Tr}(\rho\,\tilde{\chi}_{u,\delta}) + \tau_d(\delta)\,\|\rho\|\Big)\,, \tag{1.17}$$

where $\tilde{\chi}_{u,\delta} := \chi_{u,\delta}(\,\cdot+u)$ denotes the characteristic function of $B_{l(u)}(1+\delta)(0)$. If we choose Λ such that it contains the set

$$\Omega\times\Omega-(u,u) = \big\{(x-u,y-u)\in\mathbb{R}^d\times\mathbb{R}^d : x,y\in\Omega\big\}\,,$$

then $L_u(x,y) = \tilde{L}^\Lambda(x-u,y-u)\,\chi_\Omega(x)\,\chi_\Omega(y)$. Hence by (1.17)

$$\begin{aligned}\operatorname{Tr}\rho L_u &= \int\!\!\int \rho(y,x)L_u(x,y)\,dx\,dy = \int\!\!\int (\chi_\Omega\rho\chi_\Omega)(x+u,y+u)\,\tilde{L}_u^\Lambda(x,y)\,dx\,dy\\ &\leqslant\; C\,l(u)^{-1}\Big(\delta\operatorname{Tr}(\rho\,\chi_\Omega\,\chi_{u,\delta}) + \tau_d(\delta)\,\|\rho\|\Big)\,,\end{aligned}$$

since $\|\chi_\Omega\rho\chi_\Omega\|\leqslant\|\rho\|$ and $\tilde{\chi}_{u,\delta}(x-u) = \chi_{u,\delta}(x)$. This concludes the proof of (1.8). □

Proof of Proposition 5. Let $\rho\geqslant 0$ be a trace class operator with range in $H_0^{1/2}(\Omega)$. Then (see Appendix C.1), it follows from the localization formula (1.7) for the quadratic form of $A_{\mu/h}^\Omega$ that

$$\operatorname{Tr}\rho A_{\mu/h}^\Omega \;=\; \int_{\Omega^*}\Big(\operatorname{Tr}\rho\phi_u A_{\mu/h}^\Omega\phi_u - \operatorname{Tr}\rho L_u\Big)l(u)^{-d}\,du\,,$$

where L_u is the bounded integral operator with kernel (1.6) studied in Lemma 6 and 7. For each $u\in\Omega^*$ let $\delta_u\in(0,\frac12]$ to be specified later. Then, by the upper bounds on the localization error in Lemma 7,

$$\operatorname{Tr}\rho A_{\mu/h}^\Omega \;\geqslant\; \int_{\Omega^*}\operatorname{Tr}\rho\big(\phi_u A_{\mu/h}^\Omega\phi_u - C\,l(u)^{-1}\delta_u\,\chi_\Omega\,\chi_{u,\delta_u}\big)\,\frac{du}{l(u)^d} - C\,\|\rho\|\int_{\Omega^*}\tau_d(\delta_u)\,\frac{du}{l(u)^{d+1}}\,.$$

First, we want to bound the term containing the characteristic functions by a similar integral, but where $\chi_\Omega\,\chi_{u,\delta_u}$ is replaced by ϕ_u^2, so that the second term can be combined with the first term.

Following the treatment in [40] and [24], we observe the following: If for $u,u'\in\mathbb{R}^d$ there exists $x\in\operatorname{supp}\phi_{u'}\cap\operatorname{supp}\chi_{u,\delta_u}$, then $|x-u|\leqslant l(u)(1+\delta_u)$ and $|x-u'|\leqslant l(u')$. Therefore

$$|u-u'| \;\leqslant\; |u-x|+|x-u'| \;\leqslant\; l(u)(1+\delta_u)+l(u') \;\leqslant\; \tfrac32\,l(u)+l(u')\,,$$

which implies $|l(u)-l(u')|\leqslant\|\nabla l\|_\infty\,|u-u'|\leqslant\frac34\,l(u)+\frac12\,l(u')$, since $\|\nabla l\|_\infty\leqslant\frac12$. It follows that there exists $C>0$, such that for all $u,u'\in\mathbb{R}^d$

$$l(u)\leqslant C\,l(u')\,,\quad l(u')\leqslant C\,l(u)\,,\quad\text{and}\quad l(u)^{-1}\leqslant C\,l(u')^{-1}. \tag{1.18}$$

Below, we will choose δ_u such that

$$|u-u'| \;\leqslant\; \tfrac32\,l(u)+l(u') \quad\Rightarrow\quad \delta_u\leqslant C\,\delta_{u'}\,. \tag{1.19}$$

Then, by using (1.4), we get for all $x \in \mathbb{R}^d$,

$$\int_{\Omega^*} l(u)^{-1}\delta_u\, \chi_\Omega(x)\,\chi_{u,\delta_u}(x)\,\frac{du}{l(u)^d} \;=\; \int_{\Omega^*} l(u)^{-1}\delta_u\, \chi_\Omega(x)\,\chi_{u,\delta_u}(x)\bigg(\int \phi_{u'}(x)^2\frac{du'}{l(u')^d}\bigg)\frac{du}{l(u)^d}$$

$$\leqslant C\int l(u')^{-1}\,\delta_{u'}\,\chi_\Omega(x)\,\phi_{u'}(x)^2\bigg(\int_{\Omega^*}\chi_{u,\delta_u}(x)\frac{du}{l(u)^d}\bigg)\frac{du'}{l(u')^d} \;\leqslant\; C\int_{\Omega^*}\delta_{u'}\,\phi_{u'}(x)^2\frac{du'}{l(u')^{d+1}}\,.$$

Here, we have used that if $\chi_{u,\delta_u}(x)\neq 0$, then $|x-u|\leqslant l(u)(1+\delta_u)\leqslant C\,l(u')$, since $\delta_u\leqslant\frac12$ and $l(u)\leqslant C\,l(u')$, and therefore

$$\int_{\Omega^*}\chi_{u,\delta_u}(x)\,\frac{du}{l(u)^d} \;\leqslant\; C\,l(u')^{-d}\left|B_{C\,l(u')}(x)\right| \;=\; C\,.$$

It follows that

$$\operatorname{Tr}\rho A^{\Omega}_{\mu/h} \;\geqslant \int_{\Omega^*}\operatorname{Tr}\Big(\rho\phi_u\big(A^{\Omega}_{\mu/h}-C\,l(u)^{-1}\delta_u\big)\phi_u\Big)\frac{du}{l(u)^d} - C\,\|\rho\|\int_{\Omega^*}\tau_d(\delta_u)\,\frac{du}{l(u)^{d+1}}\,.$$

By using the Variational Principle (see Appendix C.2), we obtain

$$\begin{aligned}
\operatorname{Tr}\big(H^{\Omega}_{\mu,h}\big)_- \;&=\; -\inf_{0\leqslant\rho\leqslant 1}\operatorname{Tr}\rho\big(hA^{\Omega}_{\mu/h}-1\big)\\
&\leqslant\; -\inf_{0\leqslant\rho\leqslant 1}\int_{\Omega^*}\operatorname{Tr}\Big(\rho\,\phi_u\big(hA^{\Omega}_{\mu/h}-1-C\,h\,l(u)^{-1}\delta_u\big)\phi_u\Big)\,\frac{du}{l(u)^d}\\
&\qquad + C\sup_{0\leqslant\rho\leqslant 1}\|\rho\|\;h\int_{\Omega^*}\tau_d(\delta_u)\,l(u)^{-d-1}\,du\\
&\leqslant\; \int_{\Omega^*}\operatorname{Tr}\Big(\phi_u\big(H^{\Omega}_{\mu,h}-C\,h\,l(u)^{-1}\delta_u\big)\phi_u\Big)_-\,\frac{du}{l(u)^d}+C\,h\int_{\Omega^*}\tau_d(\delta_u)\,\frac{du}{l(u)^{d+1}}\,.
\end{aligned}$$

The conditions $\delta_u\leqslant\frac12$ and (1.19) are satisfied by

$$\delta_u = \begin{cases} l(u)^{-1}h & ,\quad d>2\\ l(u)^{-1}h\,|\ln(l(u)/h)|^{1/2} & ,\quad d=2\end{cases}\,, \tag{1.20}$$

due to $l(u)\geqslant\frac{l_0}{4}\geqslant 2h$ (recall that $0<h\leqslant\frac{l_0}{8}$) and (1.18). With this choice, we obtain for $d>2$ (recall that $\tau_d(\delta_u)$ was defined in (1.9))

$$\operatorname{Tr}\big(H^{\Omega}_{\mu,h}\big)_- \;\leqslant\; \int_{\Omega^*}\operatorname{Tr}\big(\phi_u\big(H^{\Omega}_{\mu,h}-C\,h^2l(u)^{-2}\big)\phi_u\big)_-\,\frac{du}{l(u)^d}+C\,h^{-d+2}\int_{\Omega^*}l(u)^{-2}\,du\,.$$

We estimate the first term by using the Variational Principle. For any family $\{\sigma_u\}_{u\in\mathbb{R}^d}$ with $0<\sigma_u\leqslant\frac12$ for all $u\in\mathbb{R}^d$, we have

$$\begin{aligned}
&\inf_{0\leqslant\rho\leqslant\mathbb{I}}\operatorname{Tr}\rho\big(\phi_u\big(H^{\Omega}_{\mu,h}-C\,h^2l(u)^{-2}\big)\phi_u\big)\\
&\geqslant(1-\sigma_u)\inf_{0\leqslant\rho\leqslant\mathbb{I}}\operatorname{Tr}\rho\phi_uH^{\Omega}_{\mu,h}\phi_u+\inf_{0\leqslant\rho\leqslant\mathbb{I}}\operatorname{Tr}\rho\big(\phi_u\big(\sigma_uH^{\Omega}_{\mu,h}-C\,h^2l(u)^{-2}\big)\phi_u\big)\,,
\end{aligned}$$

in particular, for all $u\in\mathbb{R}^d$,

$$\operatorname{Tr}\big(\phi_u\big(H^{\Omega}_{\mu,h}-C\,h^2l(u)^{-2}\big)\phi_u\big)_-\leqslant\operatorname{Tr}\big(\phi_uH^{\Omega}_{\mu,h}\phi_u\big)_-+\operatorname{Tr}\big(\phi_u\big(\sigma_uH^{\Omega}_{\mu,h}-C\,h^2l(u)^{-2}\big)\phi_u\big)_-\,.$$

If, for brevity, we set $\beta_u := \sigma_u + C h^2 l(u)^{-2}$, then it follows that

$$\begin{aligned}
&\operatorname{Tr}(H^\Omega_{\mu,h})_- - \int_{\Omega^*} \operatorname{Tr}\left(\phi_u H^\Omega_{\mu,h}\phi_u\right)_- \frac{du}{l(u)^d} \\
&\qquad \leqslant \int_{\Omega^*} \operatorname{Tr}\Big(\phi_u\big(\sigma_u h A^\Omega_{\mu/h} - \beta_u\big)\phi_u\Big)_- \frac{du}{l(u)^d} + C h^{-d+2}\int_{\Omega^*} l(u)^{-2}\,du\,. \qquad (1.21)
\end{aligned}$$

Along the same lines as in the proof of Lemma 9 (Section 2 below), by using the Variational Principle for the self-adjoint operator $\sigma_u h A^\Omega_{\mu/h} - \beta_u$, we find that

$$\begin{aligned}
\operatorname{Tr}\Big(\phi_u\big(\sigma_u h A^\Omega_{\mu/h} - \beta_u\big)\phi_u\Big)_- &\leqslant \operatorname{Tr}\Big(\phi_u\big(\sigma_u h A^{\mathbb{R}^d}_{\mu/h} - \beta_u\big)_-\phi_u\Big) \\
&= \int_{\mathbb{R}^d}\Big(\sigma_u\big(\sqrt{|2\pi hk|^2+\mu^2} - \mu\big) - \beta_u\Big)_- dk \int_{\mathbb{R}^d}\phi_u(x)^2\,dx \\
&\leqslant C\,l(u)^d\,\beta_u\int_{\mathbb{R}^d}\Big(\sqrt{\sigma_u^2|2\pi hk|^2/\beta_u^2 + \mu_u^2} - \mu_u - 1\Big)_- dk \\
&= C\,l(u)^d\,\beta_u^{1+d}\,\sigma_u^{-d}h^{-d}\int_{\mathbb{R}^d}\Big(\sqrt{|p|^2+\mu_u^2} - \mu_u - 1\Big)_- dp \\
&\leqslant C\,l(u)^d\,\beta_u^{1+d}\,\sigma_u^{-d}h^{-d}(1+\mu_u)^{d/2}\,, \qquad (1.22)
\end{aligned}$$

where $\mu_u := \mu\sigma_u/\beta_u$. Choosing $\sigma_u := h^2 l(u)^{-2}$ and recalling that $h \leqslant l_0/8$, we obtain $\sigma_u \leqslant \frac{1}{2}$, since $l(u) \geqslant l_0/4$. It follows that $\beta_u = C\sigma_u$, $\mu_u = C\mu$, and by (1.22),

$$\operatorname{Tr}\Big(\phi_u\big(\sigma_u h A^\Omega_m - \beta_u\big)\phi_u\Big)_- \leqslant C\,l(u)^{d-2}h^{-d+2}(1+\mu)^{d/2}\,.$$

Hence, by (1.21)

$$\operatorname{Tr}(H^\Omega_{\mu,h})_- - \int_{\Omega^*}\operatorname{Tr}\left(\phi_u H^\Omega_{\mu,h}\phi_u\right)_- \frac{du}{l(u)^d} \leqslant C h^{-d+2}(1+\mu)^{d/2}\int_{\Omega^*} l(u)^{-2}du\,.$$

We continue with an upper bound for $\int_{\Omega^*} l(u)^{-2}\,du$. Let $g(t) := (l_0^2 + t^2)^{-1}$, so that $l(u) = \frac{1}{2}(1 + g(\delta(u))^{1/2})^{-1}$. We have $l(u)^{-2} \leqslant 8(1+g(\delta(u)))$, i.e. we need to find an upper bound for

$$\int_{\Omega^*} g(\delta(u))\,du = \int_{\delta(\Omega^*)} g(t)\,\big(\lambda^d\circ\delta^{-1}\big)(dt)\,,$$

where λ^d denotes the Lebesgue measure on $\mathbb{R}^d$, and $\lambda^d\circ\delta^{-1}$ is the image measure of λ^d under δ. By the co-area formula [18, 3.4.2] applied to δ, we have $(\lambda^d\circ\delta^{-1})(dt) = \mathcal{H}^{d-1}(\delta^{-1}(\{t\}))\,dt$, where $\mathcal{H}^{d-1}$ denotes the $(d-1)$-dimensional Hausdorff measure (see for instance [18, Ch. 2]). By Lemma 27 in Appendix B there exists $\varepsilon > 0$ such that $\mathcal{H}^{d-1}(\delta^{-1}(\{t\})) \leqslant C$ for all $t \leqslant \varepsilon$. With $\Omega^*_\varepsilon := \{u \in \Omega^* \,|\, \delta(u) \leqslant \varepsilon\}$, we obtain

$$\begin{aligned}
\int_{\Omega^*} g(\delta(u))\,du &= \int_{\Omega^*_\varepsilon} g(\delta(u))\,du + \int_{\Omega^*\setminus\Omega^*_\varepsilon} g(\delta(u))\,du \qquad (1.23)\\
&\leqslant C\int_0^\varepsilon g(t)\,dt + \varepsilon^{-2}\int_{\Omega^*\setminus\Omega^*_\varepsilon} du \leqslant C\,l_0^{-1}\int_0^\infty \arctan'(s)\,ds + C \leqslant C\,l_0^{-1}\,,
\end{aligned}$$

and thus

$$\int_{\Omega^*} l(u)^{-2}du \leqslant C\,(1 + l_0^{-1}) \leqslant C\,l_0^{-1}\,. \qquad (1.24)$$

Hence,

$$\operatorname{Tr}\big(H^{\Omega}_{\mu,h}\big)_- - \int_{\mathbb{R}^d} \operatorname{Tr}\big(\phi_u H^{\Omega}_{\mu,h}\phi_u\big)_-\, l(u)^{-d}\, du \;\leqslant\; C\, h^{-d+2}\, l_0^{-1}(1+\mu)^{d/2}\,, \tag{1.25}$$

establishing the second inequality in (1.5) for $d > 2$. With the choice of δ_u in (1.20), the case $d = 2$ follows along the same lines (by using that $0 \leqslant \ln x \leqslant x$ whenever $x \geqslant 1$).

The lower bound in (1.5), i.e. that the left side of (1.25) is non-negative, follows from Lemma 28 and (1.4). Indeed, by (C.5),

$$\operatorname{Tr}\,(\phi_u H^{\Omega}_{\mu,h}\phi_u)_- \;\leqslant\; \operatorname{Tr}\,\phi_u (H^{\Omega}_{\mu,h})_-\phi_u \;=\; \operatorname{Tr}\,\phi_u^2 (H^{\Omega}_{\mu,h})_-\,,$$

and therefore

$$\begin{aligned}\int_{\mathbb{R}^d} \operatorname{Tr}\,(\phi_u H^{\Omega}_{\mu,h}\phi_u)_-\, l(u)^{-d} du \;&\leqslant\; \int_{\mathbb{R}^d} \sum\nolimits_{k=1}^{\infty} \big(\psi_k, \phi_u^2 (H^{\Omega}_{\mu,h})_- \psi_k\big)\, l(u)^{-d} du \\ &=\; \sum\nolimits_{k=1}^{\infty} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \phi_u^2(x)\overline{\psi_k(x)}\big[(H^{\Omega}_{\mu,h})_-\psi_k\big](x)\, dx\, l(u)^{-d} du \\ &=\; \sum\nolimits_{k=1}^{\infty} \int_{\mathbb{R}^d} \overline{\psi_k(x)}\big[(H^{\Omega}_{\mu,h})_-\psi_k\big](x)\, dx \;=\; \operatorname{Tr}\,(H^{\Omega}_{\mu,h})_-\,,\end{aligned}$$

where $(\psi_k)_{k=1}^{\infty}$ is an arbitrary orthonormal basis in $L^2(\mathbb{R}^d)$, and

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \big|\phi_u^2(x)\, \psi_k(x)\, \big[(H^{\Omega}_{\mu,h})_-\psi_k\big](x)\big|\, dx\, l(u)^{-d} du \;\leqslant\; \|\psi_k\|_2\, \big\|(H^{\Omega}_{\mu,h})_-\psi_k\big\|_2\,,$$

which allows to apply Fubini's theorem. □

2. Analysis in the bulk

We first study the case when the support of ϕ is completely contained in Ω.

Proposition 8. *There exists $C > 0$, such that for all real-valued $\phi \in C_0^1(\Omega)$ with support in a ball of radius $l > 0$, satisfying $\|\nabla\phi\|_\infty \leqslant C\, l^{-1}$,*

$$0 \;\leqslant\; \Lambda^{(1)}_{\mu}\, h^{-d}\int_{\Omega} \phi(x)^2\, dx \;-\; \operatorname{Tr}\big(\phi H^{\Omega}_{\mu,h}\phi\big)_- \;\leqslant\; C\, h^{-d+2}\, l^{d-2}\, (1+\mu)^{(d-1)/2} \tag{2.1}$$

for all $h > 0$, where $\Lambda^{(1)}_{\mu} = (2\pi)^{-d}\int_{\mathbb{R}^d} (\psi_\mu(|p|^2) - 1)_-\, dp$.

This is the analogue of [24, Prop. 4]. We prove the lower bound in Lemma 9 below, while the upper bound is an application of Lemma 10.

Lemma 9. *For any real-valued $\phi \in C_0^1(\mathbb{R}^d)$ and $h > 0$, we have*

$$\operatorname{Tr}\big(\phi H^{\Omega}_{\mu,h}\phi\big)_- \;\leqslant\; \Lambda^{(1)}_{\mu}\, h^{-d}\int_{\mathbb{R}^d} \phi(x)^2\, dx\,. \tag{2.2}$$

Proof. If we write $H_{\mu,h} := H^{\mathbb{R}^d}_{\mu,h} = hA^{\mathbb{R}^d}_{\mu/h} - 1 = \sqrt{-h^2\Delta + \mu^2} - \mu - 1$, then it follows from the Variational Principle that (see Lemma 28)

$$\operatorname{Tr}(\phi H^{\Omega}_{\mu,h}\phi)_- \;\leqslant\; \operatorname{Tr}(\phi H_{\mu,h}\phi)_- \;\leqslant\; \operatorname{Tr}\,\phi(H_{\mu,h})_-\phi\,. \tag{2.3}$$

If $\mathcal{F}$ denotes the Fourier transform on $\mathbb{R}^d$ and $\Phi := \mathcal{F}\phi\mathcal{F}^{-1}$, which is the integral operator in $L^2(\mathbb{R}^d)$ with kernel $(k, \tilde{k}) \mapsto (\mathcal{F}\phi)(k - \tilde{k})$, then we have $\operatorname{Tr}\,\phi(H_{\mu,h})_-\phi = \operatorname{Tr}\,\Phi g \Phi$, where

$g(k) := (\psi_\mu(|2\pi hk|^2)-1)_-$. Since, for any $\delta \geqslant 0$, we have

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} g(k)^\delta |\Phi(k,\tilde{k})|^2 d\tilde{k}\, dk \;=\; \int_{\mathbb{R}^d} g(k)^\delta dk\, \|\mathcal{F}\phi\|_2^2 \;<\; \infty\,,$$

it follows that the operators Φg^0 and $g\Phi$ are Hilbert-Schmidt operators, and therefore

$$\mathrm{Tr}\, \Phi g \Phi \;=\; \int_{\mathbb{R}^d} g(k)|\Phi(k,\tilde{k})|^2\, d\tilde{k}\, dk \;=\; \int_{\mathbb{R}^d} \big(\psi_\mu(|2\pi hk|^2)-1\big)_- dk\; \|\mathcal{F}\phi\|_2^2 \;=\; \Lambda_\mu^{(1)}\, h^{-d}\, \|\phi\|_2^2\,.$$

Together with (2.3), this proves (2.2). □

Lemma 10. *Let $\phi \in C_0^1(\mathbb{R}^d)$ be real-valued, $\mu, h > 0$, and $p \in \mathbb{R}^d$. Then*

$$\big\|(h\,A_{\mu/h})^{1/2}\phi e^{ip\cdot/h}\big\|_2^2 \;=\; \frac{1}{2}\int_{\mathbb{R}^d} \big(\psi_\mu(|p{+}2\pi h\eta|^2) + \psi_\mu(|p{-}2\pi h\eta|^2)\big)\, |\hat{\phi}(\eta)|^2\, d\eta\,, \tag{2.4}$$

where $A_{\mu/h} := A_{\mu/h}^{\mathbb{R}^d}$.

Proof. For $a > 0$, let ψ_μ^a be the exponential regularization of ψ_μ given by $\psi_\mu^a(E) := e^{-aE}\psi_\mu(E)$. By dominated convergence, we have

$$\begin{aligned}
\big\|(hA_{\mu/h})^{1/2}\phi e^{ip\cdot/h}\big\|_2^2 \;&=\; \int_{\mathbb{R}^d} \psi_\mu(|2\pi h\xi|^2)\, \big|\widehat{\phi e^{ip\cdot/h}}(\xi)\big|^2 d\xi \\
&= \lim_{a\to 0^+}\int_{\mathbb{R}^d} \psi_\mu^a(|2\pi h\xi|^2)\, \big|\widehat{\phi e^{ip\cdot/h}}(\xi)\big|^2 d\xi \\
&= (2\pi h)^{-d} \lim_{a\to 0^+}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \psi_\mu^a(|\xi|^2)\, e^{i(p-\xi)(x-y)/h}\phi(x)\phi(y)\, dx\, dy\, d\xi\,.
\end{aligned}$$

Since $\psi_\mu^a(|\cdot|^2) \in L^1(\mathbb{R}^d)$ for all $a > 0$, by another application of dominated convergence

$$\big\|(hA_{\mu/h})^{1/2}\phi e^{ip\cdot/h}\big\|_2^2 \;=\; \lim_{a\to 0^+}\; \lim_{b\to 0^+} \mathcal{I}_{a,b}(p)\,, \tag{2.5}$$

where

$$\mathcal{I}_{a,b}(p) \;:=\; (2\pi h)^{-d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} e^{-b|x-y|^2}\psi_\mu^a(|\xi|^2)\, e^{i(p-\xi)(x-y)/h}\phi(x)\phi(y)\, dx\, dy\, d\xi\,.$$

We write $\phi(x)\phi(y) = \frac{1}{2}\big(\phi(x)^2 + \phi(y)^2 - (\phi(x){-}\phi(y))^2\big)$, and

$$\begin{aligned}
\mathcal{I}_{a,b}^{(1)}(p) \;&:=\; (2\pi h)^{-d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} e^{-b|x-y|^2}\psi_\mu^a(|\xi|^2)\, e^{i(p-\xi)(x-y)/h}\, \frac{\phi(x)^2}{2}\, dx\, dy\, d\xi\,, \\
\mathcal{I}_{a,b}^{(2)}(p) \;&:=\; (2\pi h)^{-d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} e^{-b|x-y|^2}\psi_\mu^a(|\xi|^2)\, e^{i(p-\xi)(x-y)/h}\, \frac{\phi(y)^2}{2}\, dx\, dy\, d\xi\,, \\
\mathcal{I}_{a,b}^{(3)}(p) \;&:=\; (2\pi h)^{-d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} e^{-b|x-y|^2}\psi_\mu^a(|\xi|^2)\, e^{i(p-\xi)(x-y)/h}\, \frac{(\phi(x){-}\phi(y))^2}{2}\, dx\, dy\, d\xi\,,
\end{aligned}$$

so that

$$\mathcal{I}_{a,b}(p) \;=\; \mathcal{I}_{a,b}^{(1)}(p) + \mathcal{I}_{a,b}^{(2)}(p) - \mathcal{I}_{a,b}^{(3)}(p)\,. \tag{2.6}$$

Since $\mathcal{F}(e^{-b|\cdot|^2})(k) = (\pi/b)^{d/2}e^{-\pi^2|k|^2/b}$, by performing the dy integral in $\mathcal{I}_{a,b}^{(1)}(p)$ and the dx integral in $\mathcal{I}_{a,b}^{(2)}(p)$, it follows that

$$\mathcal{I}_{a,b}^{(1)}(p) + \mathcal{I}_{a,b}^{(2)}(p) \;=\; (2\pi h)^{-d}\Big(\frac{\pi}{b}\Big)^{d/2}\int_{\mathbb{R}^d} e^{-|p-\xi|^2/(4h^2b)}\, \psi_\mu^a(|\xi|^2)\, d\xi\, \int_{\mathbb{R}^d}\phi(x)^2\, dx\,.$$

The Gaussian functions $\beta_b := \beta_b^{(d)}$ on $\mathbb{R}^d$, given by

$$\beta_b^{(d)}(\xi) := (4h^2 b\pi)^{-d/2}\, e^{-|\xi|^2/4h^2 b}\,, \tag{2.7}$$

form an approximate identity centered at 0, in particular $\lim_{b\to 0^+}\int \beta_b(x)f(x)\,dx = f(0)$ for all $f\in C(\mathbb{R}^d)\cap L^\infty(\mathbb{R}^d)$ (see Appendix D.1). This follows from $\beta_b(x) = (2h\sqrt{b})^{-d}\beta(x/2h\sqrt{b})$, where β denotes the Gaussian $\pi^{-d/2}\,e^{-|\cdot|^2}$ satisfying $\|\beta\|_1 = 1$. Therefore, since $\psi_\mu^a(|\cdot|^2)\in \mathcal{S}(\mathbb{R}^d)\subset C(\mathbb{R}^d)\cap L^\infty(\mathbb{R}^d)$, we obtain

$$\lim_{b\to 0_+}\big(\mathcal{I}_{a,b}^{(1)}(p)+\mathcal{I}_{a,b}^{(2)}(p)\big) \;=\; \psi_\mu^a(|p|^2)\,\|\phi\|_2^2 \;=\; e^{-a|p|^2}\psi_\mu(|p|^2)\,\|\phi\|_2^2\,. \tag{2.8}$$

For $\mathcal{I}_{a,b}^{(3)}(p)$, after performing the change of variables $y\mapsto z := x-y$, we find

$$\begin{aligned}
\mathcal{I}_{a,b}^{(3)}(p) \;&=\; \frac{(2\pi h)^{-d}}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} e^{-b|z|^2}\psi_\mu^a(|\xi|^2)\,e^{i(p-\xi)z/h}\big(\phi(x)-\phi(x+z)\big)^2\,dx\,dz\,d\xi\\
&=\; \frac{(2\pi h)^{-d}}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} e^{-b|z|^2}\psi_\mu^a(|\xi|^2)\,e^{i(p-\xi)z/h}\,\big\|\mathcal{F}(\phi-\phi(\,\cdot+z))\big\|_2^2\;dz\,d\xi\\
&=\; \frac{(2\pi h)^{-d}}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} e^{-b|z|^2}\psi_\mu^a(|\xi|^2)\,e^{i(p-\xi)z/h}\,\big|1-e^{2\pi i\eta z}\big|^2\,|\hat\phi(\eta)|^2 d\eta\,dz\,d\xi\\
&=\; (2\pi h)^{-d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\psi_\mu^a(|\xi|^2)\,|\hat\phi(\eta)|^2\int_{\mathbb{R}} e^{-b|z|^2}\Big(e^{i(p-\xi)z/h}\\
&\qquad\qquad -\tfrac12\,e^{i(p-\xi+2\pi h\eta)z/h}-\tfrac12\,e^{i(p-\xi-2\pi h\eta)z/h}\Big)dz\,d\xi\,d\eta\\
&=\; \int_{\mathbb{R}}|\hat\phi(\eta)|^2\int_{\mathbb{R}}\psi_\mu^a(|\xi|^2)\Big(\beta_b(p-\xi)-\tfrac12\,\beta_b(p-\xi+2\pi h\eta)-\tfrac12\,\beta_b(p-\xi-2\pi h\eta)\Big)\,d\xi\,d\eta\,.
\end{aligned}$$

Since $\|\beta_b\|_1 = \|\beta\|_1 = 1$, it follows that $|\int_{\mathbb{R}^d}\psi_\mu^a(|\xi|^2)\beta_b(k-\xi)d\xi| \leqslant \|\psi_\mu^a\|_\infty$ uniformly in $b>0$ and $k\in\mathbb{R}^d$. Thus, by dominated convergence, we are allowed to take the limit $b\to 0_+$ inside the η-integration. We obtain

$$\lim_{b\to 0_+}\mathcal{I}_{a,b}^{(3)}(p) \;=\; \int_{\mathbb{R}}|\hat\phi(\eta)|^2\Big(\psi_\mu^a(|p|^2)-\tfrac12\psi_\mu^a(|p+2\pi h\eta|^2)-\tfrac12\psi_\mu^a(|p-2\pi h\eta|^2)\Big)\,d\eta\,. \tag{2.9}$$

Now, since $\phi\in C_0^1(\mathbb{R}^d)$ and $|\psi_\mu^a(|p\pm 2\pi h\eta|^2)|\leqslant \psi_\mu(|p\pm 2\pi h\eta|^2)\leqslant |p\pm 2\pi h\eta|$, we can use dominated convergence again, in order to take the limit $a\to 0_+$ in (2.9). Together with (2.8), it follows from (2.6) and $\|\hat\phi\|_2 = \|\phi\|_2$, that

$$\lim_{a\to 0_+}\lim_{b\to 0_+}\mathcal{I}_{a,b}(p) \;=\; \tfrac12\int_{\mathbb{R}}\big(\psi_\mu(|p+2\pi h\eta|^2)+\psi_\mu(|p-2\pi h\eta|^2)\big)\,|\hat\phi(\eta)|^2\,d\eta\,,$$

which proves the claim. □

Proof of Proposition 8. The lower bound in (2.1) is shown in Lemma 9. For the upper bound, we use Lemma 10.

Let $H_{\mu,h} = H_{\mu,h}^{\mathbb{R}^d}$, as in the proof of Lemma 9, and $\rho := \phi^0\,(H_{\mu,h})_-^0\,\phi^0$, where ϕ^0 is the characteristic function of $\operatorname{supp}\phi$. Then $0\leqslant\rho\leqslant 1$ and for all $f\in L^2(\mathbb{R}^d)$,

$$\begin{aligned}
q_\rho(f) = (f,\rho f) \;&=\; \int_{\mathbb{R}^d}\big(\psi_\mu(|2\pi hk|^2)-1\big)_-^0\;\big|\mathcal{F}(\phi^0 f)(k)\big|^2\,dk\\
&=\; (2\pi h)^{-d}\int_{\psi_\mu(|p|^2)\leqslant 1}\big|(\phi^0 e^{ip\cdot/h}, f)\big|^2\,dp\,.
\end{aligned} \tag{2.10}$$

Consequently,

$$\operatorname{Tr}\rho \;=\; (2\pi h)^{-d}\int_{\psi_\mu(|p|^2)\leqslant 1}\|e^{ip\cdot/h}\phi^0\|_2^2\,dp \;\leqslant\; (2\pi h)^{-d}\left|B^{(d)}_{\sqrt{1+2\mu}}(0)\right|\,|\operatorname{supp}\phi|^2<\infty\,.$$

Below, we show that $\sum_{j\in\mathbb{N}} q_\rho(\phi A^{1/2}_{\mu/h}\varphi_j)<\infty$ if $\{\varphi_j\}_{j\in\mathbb{N}}\subset H^{1/2}(\mathbb{R}^d)$ is an orthonormal basis in $L^2(\mathbb{R}^d)$, from which it follows for all $f\in L^2(\mathbb{R}^d)$, that

$$\sum_{j\in\mathbb{N}}|(\varphi_j,A^{1/2}_{\mu/h}\phi\rho f)|^2=\sum_{j\in\mathbb{N}}|(\rho^{1/2}\phi A^{1/2}_{\mu/h}\varphi_k,\rho^{1/2}f)|^2\leqslant\|\rho^{1/2}f\|^2\sum_{k\in\mathbb{N}}\|\rho^{1/2}\phi A^{1/2}_{\mu/h}\varphi_k\|^2<\infty\,.$$

In particular, $A^{1/2}_{\mu/h}\phi\rho f\in L^2(\mathbb{R}^d)$, i.e. $\phi\rho f\in H^{1/2}(\mathbb{R}^d)$, and thus the range of ρ belongs to the form domain of $\phi A_{\mu/h}\phi$, so that it can be used as a trial density matrix in the Variational Principle.

Since $\phi\in C^1_0(\Omega)$, the form domains of $\phi H^\Omega_{\mu,h}\phi$ and $\phi H_{\mu,h}\phi$ coincide, and therefore it follows from the Variational Principle that[9]

$$-\operatorname{Tr}\left(\phi H^\Omega_{\mu,h}\phi\right)_-\;\leqslant\;\operatorname{Tr}\rho\phi H^\Omega_{\mu,h}\phi\;=\;\operatorname{Tr}\rho\phi H_{\mu,h}\phi\;=\;h\operatorname{Tr}\rho\phi A_{\mu/h}\phi-\operatorname{Tr}\rho\phi^2. \tag{2.11}$$

In order to calculate $\operatorname{Tr}\rho\phi A_{\mu/h}\phi$, let $\{\varphi_j\}_{j\in\mathbb{N}}\subset H^{1/2}(\mathbb{R}^d)$ be an orthonormal basis in $L^2(\mathbb{R}^d)$. Then,

$$\begin{aligned}\operatorname{Tr}\rho\phi A_{\mu/h}\phi\;&=\;\sum_{j\in\mathbb{N}}\left(\phi A^{1/2}_{\mu/h}\varphi_j,\rho\phi A^{1/2}_{\mu/h}\varphi_j\right)\\&\overset{(2.10)}{=}\;(2\pi h)^{-d}\sum_{j\in\mathbb{N}}\int_{\psi_\mu(|p|^2)\leqslant 1}\left|\left(\phi^0 e^{ip\cdot/h},\phi A^{1/2}_{\mu/h}\varphi_j\right)\right|^2dp\\&=\;(2\pi h)^{-d}\int_{\psi_\mu(|p|^2)\leqslant 1}\left\|A^{1/2}_{\mu/h}\phi e^{ip\cdot/h}\right\|_2^2dp\,.\end{aligned}\tag{2.12}$$

Similarly, for $\operatorname{Tr}\rho\phi^2$ we obtain

$$\operatorname{Tr}\rho\phi^2\;=\;(2\pi h)^{-d}\int_{\psi_\mu(|p|^2)\leqslant 1}\left\|\phi e^{ip\cdot/h}\right\|_2^2dp\;=\;(2\pi h)^{-d}\|\phi\|_2^2\int_{\psi_\mu(|p|^2)\leqslant 1}dp\,. \tag{2.13}$$

From (2.11), (2.12), (2.13) and Lemma 10, it follows that

$$\begin{aligned}-\operatorname{Tr}\left(\phi H^\Omega_{\mu,h}\phi\right)_-\;&\leqslant\;(2\pi h)^{-d}\int_{\psi_\mu(|p|^2)\leqslant 1}\Big(\left\|(hA_{\mu/h})^{1/2}\phi e^{ip\cdot/h}\right\|_2^2-\|\phi\|_2^2\Big)dp\\&=\;(2\pi h)^{-d}\int_{\psi_\mu(|p|^2)\leqslant 1}\Big(\big(\psi_\mu(|p|^2)-1\big)\|\phi\|_2^2+R_{\mu,h}(p)\Big)dp\\&=\;-h^{-d}\Lambda^{(1)}_\mu\|\phi\|_2^2+(2\pi h)^{-d}\int_{\psi_\mu(|p|^2)\leqslant 1}R_{\mu,h}(p)\,dp\,,\end{aligned}\tag{2.14}$$

where

$$R_{\mu,h}(p)\;:=\;\int_{\mathbb{R}^d}\Big(\tfrac12\big(\psi_\mu(|p+2\pi h\eta|^2)+\psi_\mu(|p-2\pi h\eta|^2)\big)-\psi_\mu(|p|^2)\Big)\,|\hat\phi(\eta)|^2\,d\eta\,. \tag{2.15}$$

It remains to find a suitable upper bound for $R_{\mu,h}(p)$. We first observe that, for $a>0$ and $|b|\leqslant a$, we have $(a+b)^{1/2}+(a-b)^{1/2}\leqslant 2a^{1/2}$, since

$$\big((a+b)^{1/2}+(a-b)^{1/2}\big)^2\;=\;2a+2(a^2-b^2)^{1/2}\;\leqslant\;4a\,.$$

[9]Recall that $A_{\mu/h}:=A^{\mathbb{R}^d}_{\mu/h}$.

Applied to $a = |p|^2 + |\xi|^2 + \mu^2$ and $b = 2p \cdot \xi$, where $p, \xi \in \mathbb{R}^d$, this gives

$$\begin{aligned}
&\tfrac{1}{2}\big(\psi_\mu(|p+\xi|^2) - \psi_\mu(|p-\xi|^2)\big) - \psi_\mu(|p|^2) \\
&= \tfrac{1}{2}\Big(\big(|p+\xi|^2+\mu^2\big)^{1/2} + \big(|p-\xi|^2+\mu^2\big)^{1/2}\Big) - \big(|p|^2+\mu^2\big)^{1/2} \\
&\leqslant \big(|p|^2+|\xi|^2+\mu^2\big)^{1/2} - \big(|p|^2+\mu^2\big)^{1/2} \;\leqslant\; \tfrac{1}{2}\,|p|^{-1}|\xi|^2\,,
\end{aligned} \tag{2.16}$$

where we have used that $(c+d)^{1/2} - c^{1/2} \leqslant \frac{1}{2}c^{-1/2}d$, which holds for all $c, d > 0$ and follows from

$$0 \;\leqslant\; (c^{1/2} - (c+d)^{1/2})^2 \;=\; 2c + d + 2c^{1/2}(c+d)^{1/2}\,.$$

Hence, by (2.16),

$$\begin{aligned}
\int_{\psi_\mu(|p|^2)\leqslant 1} R_{\mu,h}(p)\,dp &\leqslant \tfrac{1}{2}(2\pi h)^2 \int_{\psi_\mu(|p|^2)\leqslant 1} |p|^{-1}dp \int_{\mathbb{R}^d} |\eta|^2|\hat{\phi}(\eta)|^2 d\eta \\
&= 2\pi^2\,h^2\;|\mathbb{S}^{d-1}| \int_0^{\sqrt{1+2\mu}} t^{d-2}\,dt\;\|\nabla\phi\|_2^2 \\
&\leqslant C\,l^{d-2}\,h^2\,(1+\mu)^{(d-1)/2}\,,
\end{aligned}$$

where we have used the assumption $\|\nabla\phi\|_\infty \leqslant Cl^{-1}$ and $|\mathrm{supp}\,(\nabla\phi)| \leqslant |B_l| \leqslant Cl^d$. Together with (2.14) this shows the upper bound in (2.1). □

3. Straightening of the boundary

In this section, we compare $H^{\Omega}_{\mu,h}$ locally near the boundary with $H^{+}_{\mu,h}$, where

$$H^{+}_{\mu,h} := H^{\mathbb{R}^d_+}_{\mu,h}\,, \quad \mathbb{R}^d_+ \;:=\; \big\{(\xi', \xi_d) \in \mathbb{R}^{d-1}{\times}\mathbb{R} \,\big|\, \xi_d > 0\big\}\,.$$

Proposition 11 below is the analogue of [24, Lemma 15]. The underlying method is referred to as *straightening of the boundary*, and relies on the assumption that the boundary is locally given by the graph of a differentiable function.

More precisely, if the support of $\phi \in C^1_0(\mathbb{R}^d)$ is contained in an open ball $B_l \subset \mathbb{R}^d$ of radius $0 < l \leqslant c$ with $B_l \cap \partial\Omega \neq 0$ and some $c > 0$ to be fixed later, we choose new coordinates in $\mathbb{R}^d$ in the following way: By translation and rotation, we can choose a Cartesian coordinate sytem centered at some $x_l \in B_l \cap \partial\Omega$, such that $(0, 1)$ is the unit inward normal vector at $x_l = (0, 0)$, where for $x \in \mathbb{R}^d$, we write $x = (x', x_d) \in \mathbb{R}^{d-1}\times\mathbb{R}$. Let

$$D_l \;:=\; \big\{x' \in \mathbb{R}^{d-1} : (x', x_d) \in B_l\big\}$$

be the projection of B_l on the hyperplane $\partial\mathbb{R}^d_+ := \{(x', x_d) \in \mathbb{R}^d : x_d = 0\}$. Since $\partial\Omega \in C^1$, for small enough $c > 0$ and $l \leqslant c$, there exists a differentiable function $g : D_l \to \mathbb{R}$, such that

$$B_l \cap \partial\Omega = \big\{(x', g(x')) : x' \in D_l\big\}\,.$$

Moreover, since $\partial\Omega$ is compact, the derivatives of the functions g for different patches along $\partial\Omega$ admit a common modulus of continuity $w : \mathbb{R}_+ \to \mathbb{R}_+$. In particular, w is non-decreasing, $w(t) \to 0$ as $t \to 0^+$, and

$$|\nabla g(x') - \nabla g(y')| \leqslant w(|x'-y'|) \tag{3.1}$$

for all $x', y' \in D_l$. If $\partial\Omega \in C^{1,\gamma}$, then there exists $C > 0$ such that $w(t) = C\, t^\gamma$. We define the diffeomorphism

$$\tau : D_l \times \mathbb{R} \to D_l \times \mathbb{R},\ (x', x_d) \mapsto \big(x', x_d - g(x')\big). \tag{3.2}$$

Then τ straightens the part of $\partial\Omega$ that lies inside of B_l, in the sense that it maps $B_l \cap \partial\Omega$ into $\partial\mathbb{R}^d_+$, since $\tau(x', g(x')) = (x', 0)$ for all $x' \in D_l$.

Proposition 11 (**Straightening of the boundary**). *There exist positive constants c and C, such that for any $\phi \in C^1_0(\mathbb{R}^d)$ with support in a ball of radius $0 < l \leqslant c$ intersecting the boundary, we have*

$$\left|\operatorname{Tr}\big(\phi H^\Omega_{\mu,h}\phi\big)_- - \operatorname{Tr}\big(\phi' H^+_{\mu,h}\phi'\big)_-\right| \ \leqslant\ C\, w(l)\, l^d (1+\mu)^{d/2} h^{-d}\,. \tag{3.3}$$

Here, $\phi' \in C^1_0(\mathbb{R}^d)$ denotes the extension of $\phi \circ \tau^{-1}$ by zero to $\mathbb{R}^d$, where τ is the diffeomorphism given in (3.2)*. Moreover,*

$$\int_\Omega \phi(x)^2\, dx \ =\ \int_{\mathbb{R}^d_+} \phi'(x)^2\, dx\,, \tag{3.4}$$

and there exists $C > 0$ such that

$$0 \ \leqslant\ \int_{\partial\Omega} \phi(x)^2 d\sigma(x) - \int_{\mathbb{R}^{d-1}} \phi'(x', 0)^2 dx' \ \leqslant\ C\, w(l)^2\, l^{d-1}\,. \tag{3.5}$$

For $\mu = 0$, (3.3) is proved in [24, Lemma 15] by using the homogeneity of $|\cdot|$. Therefore, since ψ_μ is not homogeneous for $\mu > 0$, we have to find a different strategy for the proof of

Lemma 12. *There exist positive constants c and C, such that for all $v \in H^{1/2}_0(\Omega)$ compactly supported in a ball B_l of radius $0 < l \leqslant c$, and for all $\nu > 0$,*

$$\left|q^\Omega_\nu(v) - q^+_\nu(v')\right| \ \leqslant\ C\, w(l) \min\left\{q^\Omega_\nu(v), q^+_\nu(v')\right\}, \tag{3.6}$$

where $q^+_\nu := q^{\mathbb{R}^d_+}_\nu$, and $v' \in H^{1/2}_0(\mathbb{R}^d_+)$ denotes the extension of the function $v \circ \tau^{-1}$ by zero to $\mathbb{R}^d_+$.

Proof. We start with an upper bound for the left side of (3.6) in terms of $q^+_\nu(v')$. Writing, as above, $\theta_\nu(t) = \nu^{d+1}\theta(\nu t) = (\nu/(2\pi t))^{(d+1)/2}\, K_{(d+1)/2}(\nu t) =: \theta^{(d)}_\nu(t)$, and $\Gamma_l := D_l \times \mathbb{R}$, by the integral representation (0.10),

$$\begin{aligned} q^\Omega_\nu(v) \ &=\ \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \big|v(x) - v(y)\big|^2\, \theta_\nu(|x-y|)\, dx\, dy \\ &=\ \int_{\Gamma_l}\int_{\Gamma_l} \big|v(x) - v(y)\big|^2\, \theta_\nu(|x-y|)\, dx\, dy \\ &\qquad + 2\int_{\mathbb{R}^d\setminus\Gamma_l}\int_{\Gamma_l} \big|v(x) - v(y)\big|^2\, \theta_\nu(|x-y|)\, dx\, dy \\ &=\ \int_{\Gamma_l}\int_{\Gamma_l} \big|v'(\xi) - v'(\eta)\big|^2\, \theta_\nu(|\tau^{-1}(\xi) - \tau^{-1}(\eta)|)\, d\xi\, d\eta \\ &\qquad + 2\int_{\mathbb{R}^d\setminus\Gamma_l}\int_{\Gamma_l} |v'(\xi)|^2\, \theta_\nu(|\tau^{-1}(\xi) - y|)\, d\xi\, dy\,, \end{aligned} \tag{3.7}$$

since $\operatorname{supp} v \subset \Gamma_l$, and τ has unit Jacobian determinant and is bijective on Γ_l. From the integral representation (D.5) of $K_{(d+1)/2}(\nu t)$, it follows for all $\xi, \eta \in \Gamma_l$ that

$$\begin{aligned} &\Big|\theta_\nu\big(|\tau^{-1}(\xi)-\tau^{-1}(\eta)|\big) - \theta_\nu(|\xi-\eta|)\Big| \\ &\qquad \leqslant \; \nu^{-(d+1)/2} \int_0^\infty \frac{e^{-\nu^2 u}}{(2u)^{(d+3)/2}} \Big| e^{-|\tau^{-1}(\xi)-\tau^{-1}(\eta)|^2/(4u)} - e^{-|\xi-\eta|^2/(4u)} \Big| \, du \,. \end{aligned} \tag{3.8}$$

Since $\tau^{-1}(\xi) = (\xi', \xi_d + g(\xi'))$ for all $\xi \in \Gamma_l$ we have

$$\begin{aligned} \big|\tau^{-1}(\xi)-\tau^{-1}(\eta)\big|^2 - |\xi-\eta|^2 \;&=\; 2(\xi_d-\eta_d)\big(g(\xi')-g(\eta')\big) + |g(\xi')-g(\eta')|^2 \\ &\leqslant\; 2|\xi_d-\eta_d|\,|\xi'-\eta'|\,\|\nabla g\|_\infty + |\xi'-\eta'|^2\,\|\nabla g\|_\infty^2 \\ &\leqslant\; C\,w(l)\,|\xi-\eta|^2 \,, \end{aligned} \tag{3.9}$$

where we have used that, by (3.1),

$$|\nabla g(x')| \;=\; |\nabla g(x')-\nabla g(0)| \;\leqslant\; w(|x'|) \;\leqslant\; w(l)\,, \tag{3.10}$$

for all $x' \in D_l$, and therefore $\|\nabla g\|_\infty \leqslant w(l) < 1$ for l small enough.

Since $1 - e^{-|t|} \leqslant |t|$ for all $t \in \mathbb{R}$, we obtain from (3.9) that (3.8) is bounded by

$$C\,w(l)\,|\xi-\eta|^2\,\nu^{-(d+1)/2} \int_0^\infty \frac{e^{-\nu^2 u - |\xi-\eta|^2/(4u)}}{(2u)^{(d+5)/2}}\, du \,.$$

By using the integral representation (D.5) again, we conclude that

$$\begin{aligned} \Big|\theta_\nu\big(|\tau^{-1}(\xi)-\tau^{-1}(\eta)|\big) - \theta_\nu(|\xi-\eta|)\Big| \;&\leqslant\; C\,w(l)\,\nu\,|\xi-\eta|^2 \theta_\nu^{(d+2)}(|\xi-\eta|) \\ &=\; C\,w(l)\,\nu\,|\xi-\eta|\,K_{(d+3)/2}(\nu|\xi-\eta|)/|\xi-\eta|^{(d+1)/2} \\ &\leqslant\; C\,w(l)\,\theta_\nu(|\xi-\eta|/\sqrt{2})\,, \end{aligned} \tag{3.11}$$

where we have used Lemma 32 (based on the integral representation (D.7) in Appendix D.2), by which it follows that

$$\nu\,|\xi-\eta|\,K_{(d+3)/2}(\nu|\xi-\eta|) \;\leqslant\; 2\,K_{(d+1)/2}\big(\nu|\xi-\eta|/\sqrt{2}\big)\,.$$

Next, considering the second term in (3.7), containing $\theta_\nu(|\tau^{-1}(\xi)-y|)$ with $\xi \in \Gamma_l$ and $y \in \mathbb{R}^d\backslash\Gamma_l$, we have

$$\begin{aligned} &\Big|\theta_\nu\big(|\tau^{-1}(\xi)-y|\big) - \theta_\nu(|\xi-y|)\Big| \\ &\qquad \leqslant \; \nu^{-(d+1)/2} \int_0^\infty \frac{e^{-\nu^2 u}}{(2u)^{(d+3)/2}} \Big| e^{-|\tau^{-1}(\xi)-y|^2/(4u)} - e^{-|\xi-y|^2/(4u)} \Big| \, du \,. \end{aligned} \tag{3.12}$$

As above, from $\tau^{-1}(\xi) = (\xi', \xi_d + g(\xi'))$ and $y = (y', y_d)$, it follows that

$$\begin{aligned} |\tau^{-1}(\xi)-y|^2 - |\xi-y|^2 \;&=\; 2(\xi_d-y_d)g(\xi') + |g(\xi')|^2 \\ &=\; 2(\xi_d-y_d)\big(g(\xi')-g(0)\big) + \big|g(\xi')-g(0)\big|^2 \\ &\leqslant\; 2(\xi_d-y_d)|\xi'-y'|\,\|\nabla g\|_\infty + |\xi'-y'|^2\|\nabla g\|_\infty^2 \\ &\leqslant\; C\,w(l)\,|\xi-y|^2 \;. \end{aligned}$$

Therefore, as above, it follows that

$$\Big|\theta_\nu\big(|\tau^{-1}(\xi)-y|\big) - \theta_\nu\big(|\xi-y|\big)\Big| \;\leqslant\; C\,w(l)\,\theta_\nu\big(|\xi-y|/\sqrt{2}\big)\,. \tag{3.13}$$

By using (3.11) and (3.13) in (3.7), it follows that

$$\begin{aligned}
&\Big|q_\nu^\Omega(v) - q_\nu^+(v')\Big| \\
&\quad\leqslant \Big(\frac{\nu}{2\pi}\Big)^{(d+1)/2}\int_{\Gamma_l}\int_{\Gamma_l} \big|v'(\xi)-v'(\eta)\big|^2 \Big|\theta_\nu\big(|\tau^{-1}(\xi)-\tau^{-1}(\eta)|\big) - \theta_\nu\big(|\xi-\eta|\big)\Big|\, d\xi\, d\eta \\
&\qquad + 2\Big(\frac{\nu}{2\pi}\Big)^{(d+1)/2}\int_{\mathbb{R}^d\setminus\Gamma_l}\int_{\Gamma_l} |v'(\xi)|^2 \Big|\theta_\nu\big(|\tau^{-1}(\xi)-y|\big) - \theta_\nu\big(|\xi-y|\big)\Big|\, d\xi\, dy\,, \\
&\quad\leqslant C\,w(l)\Big(\frac{\nu}{2\pi}\Big)^{(d+1)/2}\int\int \big|v'(\xi)-v'(\eta)\big|^2\theta_\nu\big(|\xi-\eta|/\sqrt{2}\big)\, d\xi\, d\eta \;=\; C\,w(l)\, q^+_{\nu/\sqrt{2}}(v')\,.
\end{aligned}$$

Hence, for all $f \in H_0^{1/2}(\mathbb{R}^d_+)$,

$$q^+_{\nu/\sqrt{2}}(f) \;=\; \tfrac{1}{\sqrt{2}}\int_{\mathbb{R}^d} \psi_\nu(2|2\pi k|^2)\, |\hat{f}(k)|^2\, dk \;\leqslant\; \sqrt{2}\, q_\nu^+(f)\,.$$

Note that the property $\psi_\nu(2\lambda) \leqslant 2\psi_\nu(\lambda)$ for all $\lambda > 0$, which we used in this inequality, is shared with a special class of functions called *Bernstein functions*[10]. This follows from the fact that Bernstein functions are negative definite in the sense of Bochner, which means that the real symmetric matrix $(a_{j,k})_{j,k=1}^n$, given by $a_{j,k} = \psi(s_j)+\psi(s_k)-\psi(s_j+s_k)$, is positive definite for any choice of $s_1, \ldots, s_n > 0$ and all $n \in \mathbb{N}$. In fact, ψ_ν is a Bernstein function (see Appendix E.7).

By changing the roles of q_ν^Ω and q_ν^+, i.e. by starting with $q_\nu^+(v')$ and changing variables from $\xi = \tau(x)$ to x, we can follow the same lines as above, expect for the replacement of τ^{-1} by τ, which means a switch of the sign of g, and this does not change the result. □

Proof of Proposition 11. First, as in [24, Lemma 15], (3.4) and (3.5) immediately follow from a change of variables and (3.10).

Let $\phi \in C_0^1(B_l)$, where B_l is a ball of radius $l > 0$ intersecting the boundary. From the Variational Principle, it follows that

$$-\operatorname{Tr}(\phi H^\Omega_{\mu,h}\phi)_- \;=\; \inf_{0\leqslant\rho\leqslant 1} \operatorname{Tr}\rho\phi H^\Omega_{\mu,h}\phi\,, \tag{3.14}$$

where the infimum is taken in the set of all trace class operators ρ with $0 \leqslant \rho \leqslant 1$ and range in the form domain of $\phi H^\Omega_{\mu,h}\phi$. If $\rho = \sum_{k\in I}\mu_k(\psi_k,\cdot)\psi_k$ is the singular value decomposition of such a trial density matrix, then in view of (C.3), we have

$$\operatorname{Tr}\rho\phi H^\Omega_{\mu,h}\phi \;=\; \sum\nolimits_{k\in I}\mu_k\Big(h\, q^\Omega_{\mu/h}(\phi\psi_k) - \|\phi\psi_k\|_2^2\Big)\,,$$

since $\psi \mapsto q^\Omega_{\mu/h}(\phi\psi)$ is the quadratic form of $\phi A^\Omega_{\mu/h}\phi$. Therefore, without loss of generality we may assume that the ψ_k's are supported in $B_l \cap \Omega$. For $l \leqslant c$ with c small enough such that the diffeomorphism (3.2) is defined, let $\psi'_k \in H_0^{1/2}(\mathbb{R}^d_+)$ denote the extension of $\psi_k\circ\tau^{-1}$ by zero to $\mathbb{R}^d$, so that $\rho' := \sum_{k\in I}\mu_k(\psi'_k,\cdot)\psi'_k$ has range in $H_0^{1/2}(\mathbb{R}^d_+)$, the form domain of $\phi' H_m^+\phi'$.

By Lemma 12, there exists a constant $C > 0$ only depending on Ω and the dimension d, such that for all $k \in I$

$$q^\Omega_{\mu/h}(\phi\psi_k) \;\geqslant\; \big(1-Cw(l)\big)\, q^+_{\mu/h}(\phi'\psi'_k)\,. \tag{3.15}$$

[10]See Appendix E.3 for the definition of Bernstein functions and some basic properties.

Hence, together with $\|\phi\psi_k\|_2 = \|\phi'\psi_k'\|_2$ (τ has unit Jacobian determinant), we obtain

$$\begin{aligned} \operatorname{Tr}\rho\phi H^{\Omega}_{\mu,h}\phi \ &\geqslant\ \sum\nolimits_{k\in I}\mu_k\Big(h(1{-}Cw(l))q^{+}_{\mu/h}(\phi'\psi_k') - \|\phi'\psi_k'\|_2^2\Big) \\ &=\ \operatorname{Tr}\rho'\phi'\Big(h\big(1{-}Cw(l)\big)A^{+}_{\mu/h} - 1\Big)\phi'\,. \end{aligned}$$

By the Variational Principle and (3.14), this shows that

$$\operatorname{Tr}(\phi H^{\Omega}_{\mu,h}\phi)_- \ \leqslant\ \operatorname{Tr}\Big(\phi'\Big(h\big(1{-}Cw(l)\big)A^{+}_{\mu/h} - 1\Big)\phi'\Big)_- \ . \tag{3.16}$$

By inequality (**??**) with $A = \phi'(hA^{+}_{\mu/h}{-}1)\phi'$ and $B = Cw(l)h\,\phi' A^{+}_{\mu/h}\phi'$, for any positive parameter $\varepsilon \leqslant 1/2$,

$$\Big(\phi'\Big(h\big(1-Cw(l)\big)A^{+}_{\mu/h} - 1\Big)\phi'\Big)_- \ \leqslant\ \Big(\phi'(hA^{+}_{\mu/h}{-}1)\phi'\Big)_- + \Big(\phi'\big((\varepsilon{-}Cw(l))hA^{+}_{\mu/h} - \varepsilon\big)\phi'\Big)_- \,.$$

Hence, for c small enough such that $\varepsilon := 2Cw(l) \leqslant 1/2$ for all $0 < l \leqslant c$, it follows that

$$\operatorname{Tr}\big(\phi H^{\Omega}_{\mu,h}\phi\big)_- \ \leqslant\ \operatorname{Tr}\big(\phi' H^{+}_{\mu,h}\phi'\big)_- + 2Cw(l)\operatorname{Tr}\Big(\phi'\big(\tfrac{h}{2}A^{+}_{\mu/h}{-}1\big)\phi'\Big)_- \,. \tag{3.17}$$

In order to bound the second term on the right side of this inequality, we observe that the proof of Lemma 9 (Section 2) does not depend on the boundedness of the domain Ω. In fact, replacing $H^{\Omega}_{\mu,h}$ by $H^{+}_{\mu/2,h/2} = \frac{h}{2}A^{+}_{\mu/h}{-}1$, does not change any of the inequalities, besides a constant factor. Thus,

$$\operatorname{Tr}\big(\phi'\big(\tfrac{h}{2}A^{+}_{\mu/h}{-}1\big)\phi'\big)_- \ \leqslant\ 2^d\Lambda^{(1)}_{\mu/2}h^{-d}\,\|\phi\|_2^2\,, \tag{3.18}$$

where

$$\Lambda^{(1)}_{\mu/2} \ =\ (2\pi)^{-d}\int(\psi_{\mu/2}(|p|^2){-}1)_- dp \ \leqslant C\,(1{+}\mu)^{d/2}\ .$$

Since $\operatorname{supp}(\phi) \subset B_l$, it follows from (3.18) that

$$\operatorname{Tr}\big(\phi'\big(\tfrac{h}{2}A^{+}_{\mu/h}{-}1\big)\phi'\big)_- \ \leqslant\ C l^d(1{+}\mu)^{d/2}h^{-d}\,. \tag{3.19}$$

From (3.19) and (3.17), we obtain

$$\operatorname{Tr}\big(\phi H^{\Omega}_{\mu,h}\phi\big)_- - \operatorname{Tr}\big(\phi' H^{+}_{\mu,h}\phi'\big)_- \ \leqslant\ C\,w(l)\,l^d(1{+}\mu)^{d/2}h^{-d}\,.$$

By interchanging the roles of $H^{\Omega}_{\mu,h}$ and $H^{+}_{\mu,h}$ in the proof above, we obtain (3.3). This is due to the symmetry of the inequality in Lemma 12 under this replacement, which leads to the key inequality (3.15). ☐

4. From the half-space to the half-line

In this section, the analysis of $\operatorname{Tr}(\phi H^{+}_{\mu,h}\phi)_-$ for $\phi \in C^1_0(\mathbb{R}^d)$ is reduced to a problem on the half-line (Proposition 15 below). Following [24, Section 3.2], we define a unitary operator from $L^2(\mathbb{R}^d_+)$ to the constant fiber direct integral space $\int^{\oplus}_{\mathbb{R}^{d-1}} L^2(\mathbb{R}_+) := L^2(\mathbb{R}^{d-1}; L^2(\mathbb{R}_+))$ [46, XIII.16]. This allows to express $A^{+}_{\mu/h}$ in terms of a family of one-dimensional model operators $\{T^{+}_{\omega}\}_{\omega\geqslant 0}$, for which we will apply the diagonalization results by Kwaśnicki [37] in the next section.

Let $\mathcal{F}^{(d-1)}$ denote the partial Fourier transform of $f \in L^2(\mathbb{R}^d)$ in the first $d{-}1$ variables,

$$\mathcal{F}^{(d-1)} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d),\ (\mathcal{F}^{(d-1)}f)(\xi',\xi_d) := \big(\mathcal{F}f(\cdot,\xi_d)\big)(\xi')\,, \tag{4.1}$$

for almost all $\xi' \in \mathbb{R}^{d-1}$ and $\xi_d \in \mathbb{R}$, where $\mathcal{F}$ denotes Fourier transform in $L^2(\mathbb{R}^{d-1})$. Also, for $g \in \int^{\oplus}_{\mathbb{R}^{d-1}} L^2(\mathbb{R}_+)$ and $\xi' \in \mathbb{R}^{d-1}$, we use the notation $g_{\xi'} := g(\xi') \in L^2(\mathbb{R}_+)$.

Lemma 13. *The operator* $U : L^2(\mathbb{R}^d_+) \to \int^{\oplus}_{\mathbb{R}^{d-1}} L^2(\mathbb{R}_+)$*, given by*

$$(Uf)_{\xi'}(t) \ := \ |2\pi\xi'|^{-1/2}\big(\mathcal{F}^{(d-1)}f\big)(\xi', |2\pi\xi'|^{-1}t) \tag{4.2}$$

for almost all $\xi' \in \mathbb{R}^{d-1}$ *and* $t > 0$*, is unitary.*

Proof. By the unitarity of the Fourier transform, U is invertible, and moreover the change of variables $(\xi', \xi_d) \mapsto (\xi', t) = (\xi', |2\pi\xi'|\xi_d)$ yields

$$\begin{aligned} \|f\|^2_{L^2(\mathbb{R}^d_+)} \ &= \ \int_{\mathbb{R}^{d-1}} \int_{\mathbb{R}_+} \big|\mathcal{F}^{(d-1)} f(\xi', \xi_d)\big|^2 \, d\xi_d \, d\xi' \\ &= \ \int_{\mathbb{R}^{d-1}} \int_{\mathbb{R}_+} |2\pi\xi'|^{-1} \big|\mathcal{F}^{(d-1)} f(\xi', |2\pi\xi'|^{-1}t)\big|^2 \, dt \, d\xi' \\ &= \ \int_{\mathbb{R}^{d-1}} \|(Uf)_{\xi'}\|^2_{L^2(\mathbb{R}_+)} \, d\xi' \ = \ \|Uf\|^2_{\int^{\oplus}_{\mathbb{R}^{d-1}} L^2(\mathbb{R}_+)} \ , \end{aligned}$$

i.e. U is also an isometry. □

This leads to a representation of $q^+_{\mu/h}$, the quadratic form of $A^+_{\mu/h}$, in terms of a family of quadratic forms Q^+_ω on $L^2(\mathbb{R}_+)$.

Lemma 14. *For* $\omega \geqslant 0$*, let* Q^+_ω *denote the closed quadratic form with domain* $H^{1/2}_0(\mathbb{R}_+)$ *and*

$$Q^+_\omega(u) \ := \ \int_{\mathbb{R}} \psi_\omega\big((2\pi s)^2 + 1\big) \, |\hat{u}(s)|^2 \, ds \, , \tag{4.3}$$

where, by (0.9)*,* $\psi_\omega(E) = \sqrt{E + \omega^2} - \omega$ *for* $E \geqslant 0$*. Then if* U *denotes the unitary operator defined in Lemma 13, we have for all* $f \in H^{1/2}_0(\mathbb{R}^d_+)$ *that*

$$q^+_{\mu/h}(f) = \int_{\mathbb{R}^{d-1}} |2\pi\xi'| \, Q^+_{\mu/|2\pi h\xi'|}\Big((Uf)_{\xi'}\Big) \, d\xi' \, . \tag{4.4}$$

Proof. The claim follows from the scaling properties of ψ_ω and the Fourier transform. Indeed, for $\omega, \nu, t > 0$, we have $\psi_\omega(\nu^2 t) = \nu \, \psi_{\omega/\nu}(t)$. Moreover, for $u \in L^2(\mathbb{R})$, and $\omega, s > 0$, we have $\big(\mathcal{F}u(\omega^{-1}\cdot)\big)(s) = \omega \, (\mathcal{F}u)(\omega s)$. Hence, it follows that

$$\begin{aligned} \int_{\mathbb{R}^d} \psi_{\mu/h}(|2\pi k|^2) \, |\hat{f}(k)|^2 \, dk \ &= \ \int_{\mathbb{R}^{d-1}} \int_{\mathbb{R}} \psi_{\mu/h}\big((2\pi)^2(|\xi'|^2 + \xi_d^2)\big) \, \big|\hat{f}(\xi', \xi_d)\big|^2 \, d\xi_d \, d\xi' \\ &= \ \int_{\mathbb{R}^{d-1}} |2\pi\xi'| \int_{\mathbb{R}} \psi_{\mu/|2\pi h\xi'|}\big((\xi_d/|\xi'|)^2 + 1\big) \, \big|\hat{f}(\xi', \xi_d)\big|^2 \, d\xi_d \, d\xi' \\ &= \ \int_{\mathbb{R}^{d-1}} |2\pi\xi'|^2 \int_{\mathbb{R}} \psi_{\mu/|2\pi h\xi'|}\big((2\pi s)^2 + 1\big) \, \big|\hat{f}(\xi', |2\pi\xi'|s)\big|^2 \, ds \, d\xi' \, . \end{aligned}$$

By the scaling property of the Fourier transform, we have for almost all $\xi' \in \mathbb{R}^{d-1}$ that

$$(\mathcal{F}(Uf)_{\xi'})(s) \ = \ |2\pi\xi'|^{-1/2} \mathcal{F}\big(\mathcal{F}^{(d-1)} f(\xi', |2\pi\xi'|^{-1} \cdot)\big)(s) \ = \ |2\pi\xi'|^{1/2} \hat{f}(\xi', |2\pi\xi'|s) \, .$$

Hence

$$\int_{\mathbb{R}^d} \psi_{\mu/h}(|2\pi k|^2) \, |\hat{f}(k)|^2 \, dk \ = \ \int_{\mathbb{R}^{d-1}} |2\pi\xi'| \int_{\mathbb{R}} \psi_{\mu/|2\pi h\xi'|}\big((2\pi s)^2 + 1\big) \, \big|(\mathcal{F}(Uf)_{\xi'})(s)\big|^2 \, ds \, d\xi' \, ,$$

which proves (4.4). □

For $h > 0$, let S_h be the unitary scaling operator in $\int_{\mathbb{R}^{d-1}}^{\oplus} L^2(\mathbb{R}_+)$ given by

$$(S_h g)_{\xi'}(t) = (2\pi h)^{-(d-1)/2} g_{\xi'/2\pi h}(t)\,,$$

and let $U_h := S_h \circ U$. Then, from (4.4) it follows that for all $f \in H_0^{1/2}(\mathbb{R}^d_+)$,

$$h\, q^+_{\mu/h}(f) \;=\; \int_{\mathbb{R}^{d-1}} |\xi'|\, Q^+_{\mu/|\xi'|}\Big((U_h f)_{\xi'}\Big)\, d\xi'\,. \tag{4.5}$$

For $\omega \geqslant 0$, let T^+_ω denote the self-adjoint operator in $L^2(\mathbb{R}_+)$ given by the closed quadratic form Q^+_ω, i.e. $T^+_\omega = \psi_\omega\big(-\frac{d^2}{dt^2}+1\big)$ with Dirichlet boundary condition on $\mathbb{R}_+$.

According to [46, Theorem XIII.85], if $B_{\xi'} := |\xi'| T^+_{\mu/|\xi'|}$ then the operator $B =: \int_{\mathbb{R}^{d-1}}^{\oplus} B_{\xi'}\, d\xi'$ in $\int_{\mathbb{R}^{d-1}}^{\oplus} L^2(\mathbb{R}_+)$, with domain

$$\mathcal{D}(B) \;=\; \Big\{ g \in \textstyle\int_{\mathbb{R}^{d-1}}^{\oplus} L^2(\mathbb{R}_+) \;\Big|\; g_{\xi'} \in \mathcal{D}(B_{\xi'}) \text{ a.e.}, \int_{\mathbb{R}^{d-1}} \|B_{\xi'} g_{\xi'}\|^2_{L^2(\mathbb{R}_+)} d\xi' < \infty \Big\}\,, \tag{4.6}$$

and $(Bg)_{\xi'} := B_{\xi'} g_{\xi'}$, is self-adjoint, and since $B_{\xi'}$ is positive semidefinite, also B is positive semidefinite. Moreover, for the corresponding quadratic forms q_B and $q_{B_{\xi'}} = |\xi'| Q^+_{\mu/|\xi'|}$, we have that $g \in \mathcal{D}(q_B)$ if and only if $g_{\xi'} \in \mathcal{D}(q_{B_{\xi'}}) = H_0^{1/2}(\mathbb{R}_+)$ for almost all ξ' and

$$q_B(g) \;=\; \int_{\mathbb{R}^{d-1}} q_{B_{\xi'}}(g_{\xi'})\, d\xi' \;<\; \infty\,. \tag{4.7}$$

As a consequence of Lemma 14, this terminology may be used in order to deduce the following direct integral representation of $hA^+_{\mu/h}$ in $\int_{\mathbb{R}^{d-1}}^{\oplus} L^2(\mathbb{R}_+)$.

Proposition 15. *If T^+_ω denotes the self-adjoint operator in $L^2(\mathbb{R})$ generated by the quadratic form Q^+_ω defined in Lemma 14, and $U_h = S_h \circ U$ as above, then*

$$U_h\, hA^+_{\mu/h}\, U_h^* \;=\; \int_{\mathbb{R}^{d-1}}^{\oplus} |\xi'| T^+_{\mu/|\xi'|}\, d\xi'\,. \tag{4.8}$$

Moreover, for all bounded Borel functions Θ on $\mathbb{R}$,

$$U_h\, \Theta(hA^+_{\mu/h}) U_h^* \;=\; \int_{\mathbb{R}^{d-1}}^{\oplus} \Theta\big(|\xi'| T^+_{\mu/|\xi'|}\big)\, d\xi'\,. \tag{4.9}$$

Proof. From (4.7) and $q_{B_{\xi'}} = |\xi'| Q^+_{\mu/|\xi'|}$, it follows that the right side of (4.5) is the quadratic form of $B = \int_{\mathbb{R}^{d-1}}^{\oplus} |\xi'| T^+_{\mu/|\xi'|}\, d\xi'$, evaluated in $U_h f \in \int_{\mathbb{R}^{d-1}}^{\oplus} L^2(\mathbb{R}_+)$. In particular, (4.5) and (4.7) imply that $\mathcal{D}(q_B) = \mathcal{D}(q^+_{\mu/h}) = H_0^{1/2}(\mathbb{R}^d_+)$. Hence, both sides of (4.8) are self-adjoint positive semidefinite operators generated by the same closed quadratic form, and therefore coincide.

Equation (4.9) then follows from the fact that $\Theta(U_h A^+_{\mu/h} U_h^*) = U_h \Theta(A^+_{\mu/h}) U_h^*$, and from

$$\Theta\Big(\int_{\mathbb{R}^{d-1}}^{\oplus} |\xi'| T^+_{\mu/|\xi'|}\, d\xi' \Big) \;=\; \int_{\mathbb{R}^{d-1}}^{\oplus} \Theta\big(|\xi'| T^+_{\mu/|\xi'|}\big)\, d\xi'\,,$$

which is a consequence of [46, Theorem XIII.85 (c)]. □

5. Model operators on the half-line

In this section we study the one-dimensional model operators T^+_ω by applying the results [37] by Kwaśnicki, which provide an explicit spectral representation of the generators of a class of stochastic processes on the half-line. Therefore, in the following discussion, we use terminology from the theory of stochastic processes. Appendix E presents the relevant ideas in a concise form, including references to given statements.

Theorem 1.1 and Theorem 1.3 in [37] give a generalized eigenfunction expansion of the generator of a symmetric one-dimensional Lévy process X killed upon exiting the half-line, with Lévy exponent of the form $\eta(\xi) = f(\xi^2)$, where f is a so called *complete Bernstein function* satisfying $\lim_{t\to 0^+} f(t) = 0$. As is discussed in Appendix E.4, such processes are called *subordinated* to Brownian motion on the real line, which is characterized by the Lévy exponent $\xi \mapsto \xi^2$. The concept of killing the process when leaving the half-line corresponds to the Dirichlet boundary condition of the associated generator (see Appendix E.2).

Lemma 16 (Results from [37])**.** *For a complete Bernstein function f with $f(0+) = 0$, let A be the generator in $L^2(\mathbb{R}_+)$ of the Lévy process X with Lévy exponent $\xi \mapsto f(\xi^2)$ killed upon leaving $(0,\infty)$, and let $(P_s)_{s\geqslant 0}$ denote the contraction semigroup associated to X. Then there exists a unitary operator Π in $L^2(\mathbb{R}_+)$ such that $\Pi P_s \Pi^*$ is the operator of multiplication by $e^{-sf(\lambda^2))}$ for all $s \geqslant 0$, and $g \in L^2(\mathbb{R}_+)$ belongs to $\mathcal{D}(A)$ if and only if the function $\lambda \mapsto f(\lambda^2)\Pi g(\lambda)$ belongs to $L^2(\mathbb{R}_+)$, in which case*

$$\Pi A g(\lambda) \;=\; -f(\lambda^2)\Pi g(\lambda) \tag{5.1}$$

for all $\lambda > 0$. Moreover, for $\phi \in L^1(0,\infty) \cap L^2(\mathbb{R}_+)$ we have

$$\Pi\phi(\lambda) \;=\; \sqrt{\frac{2}{\pi}} \int_0^\infty F_\lambda(t)\,\phi(t)\,dt\,, \tag{5.2}$$

where F_λ are bounded differentiable functions of the form

$$F_\lambda(t) \;=\; \sin\big(\lambda t + \vartheta(\lambda)\big) + G_\lambda(t)\,. \tag{5.3}$$

Here, ϑ is given by

$$\vartheta(\lambda) \;:=\; \frac{1}{\pi}\int_0^\infty \frac{\lambda}{s^2-\lambda^2}\,\ln\frac{(\lambda^2-s^2)f'(\lambda^2)}{f(\lambda^2)-f(s^2)}\;ds\;, \tag{5.4}$$

and G_λ is the Laplace transform of a finite measure on $(0,\infty)$, satisfying

$$0 \;\leqslant\; G_\lambda(t) \;\leqslant\; \sin\vartheta(\lambda) \tag{5.5}$$

and

$$\int_0^\infty e^{-tx}\,G_\lambda(x)\,dx \;=\; \frac{\lambda\cos\vartheta(\lambda) + t\sin\vartheta(\lambda)}{\lambda^2+t^2} - \frac{\lambda^2}{\lambda^2+t^2}\sqrt{\frac{f'(\lambda^2)}{f(\lambda^2)}}\,\varphi_\lambda(t)\,, \tag{5.6}$$

where

$$\varphi_\lambda(t) \;:=\; \exp\left(\frac{1}{\pi}\int_0^\infty \frac{t}{t^2+s^2}\,\ln\frac{1-s^2/\lambda^2}{1-f(s^2)/f(\lambda^2)}\;ds\right) \tag{5.7}$$

for all $t \geqslant 0$ and $\lambda > 0$.

Proof. The main part of the lemma is [37, Theorem 1.3]. Inequality (5.5) is proved in [37, Lemma 4.21] and (5.6) is due to [37, (4.11)] and [37, Proposition 4.7]. □

Corollary 17 (Spectral representation of T_ω^+)**.** *For fixed $\omega \geqslant 0$ and all $\lambda > 0$ there exists a real-valued differentiable function $F_{\omega,\lambda}$ on $(0,\infty)$ satisfying $|F_{\omega,\lambda}(x)| \leqslant 2$ for all $x, \lambda \in (0,\infty)$, such that the operator Π_ω defined by* (5.2) *extends to a unitary operator in $L^2(\mathbb{R}_+)$, and $g \in \mathcal{D}(T_\omega^+)$ if and only if the function $\lambda \mapsto \psi_\omega(\lambda^2{+}1)\Pi_\omega g(\lambda)$ is in $L^2(\mathbb{R}_+)$. In this case,*

$$\Pi_\omega T_\omega^+ g(\lambda) \;=\; \psi_\omega(\lambda^2{+}1)\,\Pi_\omega g(\lambda) \qquad \text{for all } \lambda > 0. \tag{5.8}$$

More precisely, $F_{\omega,\lambda}$ has the form (5.3) *with the phase shift*

$$\vartheta_\omega(\lambda) \;=\; \frac{1}{\pi}\int_0^\infty \frac{\lambda}{s^2-\lambda^2}\;\ln\left(\frac{1}{2}+\frac{1}{2}\sqrt{\frac{s^2{+}1{+}\omega^2}{\lambda^2{+}1{+}\omega^2}}\right)ds \;=\; \vartheta_0\left(\frac{\lambda}{\sqrt{1{+}\omega^2}}\right). \tag{5.9}$$

Proof. We apply Lemma 16 to the complete Bernstein function f_ω given by

$$f_\omega(t) := \psi_\omega(t{+}1) - \psi_\omega(1) \;=\; \sqrt{t{+}1{+}\omega^2} - \sqrt{1{+}\omega^2} \quad \forall t > 0\,, \tag{5.10}$$

and satisfying $\lim_{t\to 0^+} f_\omega(t) = f_\omega(0) = 0$. If T denotes the $L^2(\mathbb{R}_+)$ generator of the subordinated Lévy process with Lévy symbol $\lambda \to f_\omega(\lambda^2)$ killed upon leaving $(0,\infty)$, then $-T = T_\omega^+ - \psi_\omega(1)$ (compare Appendix E.5). Therefore, (5.8) is an immediate consequence of (5.1). Moreover, by (5.5), $|F_{\omega,\lambda}(x)| \leqslant 2$. □

The following Lemma provides basic properties of ϑ_ω and its first two derivatives.

Lemma 18 (Properties of ϑ_ω)**.** *For each $\omega \geqslant 0$, the function ϑ_ω is monotonically increasing, and twice differentiable on $(0,\infty)$. Moreover,*

$$\frac{d\vartheta_\omega}{d\lambda}(\lambda) \;\leqslant\; \frac{1}{\pi}\frac{\sqrt{1{+}\omega^2}}{\lambda^2{+}1{+}\omega^2}\;, \quad \left|\frac{d^2\vartheta_\omega}{d\lambda^2}(\lambda)\right| \;\leqslant\; \frac{3}{\pi}\frac{\sqrt{1{+}\omega^2}}{(\lambda^2{+}1{+}\omega^2)^{3/2}} \tag{5.11}$$

for all $\lambda > 0$, and

$$\lim_{\lambda\to 0^+}\vartheta_\omega(\lambda) = 0, \quad \lim_{\lambda\to\infty}\vartheta_\omega(\lambda) = \frac{\pi}{8}, \quad \lim_{\lambda\to 0^+}\vartheta'_\omega(\lambda) = \frac{1}{\pi\sqrt{1{+}\omega^2}}. \tag{5.12}$$

Proof. Due to the scaling property $\vartheta_\omega(\lambda) = \vartheta_0(\lambda/\sqrt{1{+}\omega^2})$, we can recover the properties of ϑ_ω from those of ϑ_0.

In [37, Prop 4.17] it is proved that, for any complete Bernstein function f, the phase shift (5.4) is differentiable, and furthermore that it may be differentiated under the integral sign. Let $l_\omega(s,\lambda)$ denote the logarithm in (5.9). Since $\partial_\lambda(\lambda/(s^2{-}\lambda^2)) = (s^2{+}\lambda^2)/(s^2{-}\lambda^2)^2$ is symmetric with respect to an interchange of λ and s, integrating by parts yields

$$\begin{aligned}
\frac{d\vartheta_0}{d\lambda}(\lambda) \;&=\; \frac{1}{\pi}\int_0^\infty \left[-\frac{s}{\lambda^2-s^2}\frac{\partial}{\partial s}l_0(s,\lambda) \;+\; \frac{\lambda}{s^2-\lambda^2}\frac{\partial}{\partial\lambda}l_0(s,\lambda)\right]ds \\
&=\; \frac{1}{\pi}\int_0^\infty \frac{s}{s^2-\lambda^2}\left(1+\sqrt{\frac{s^2{+}1}{\lambda^2{+}1}}\right)^{-1}\frac{s}{\sqrt{\lambda^2{+}1}\sqrt{s^2{+}1}}\,ds \\
&\quad + \frac{1}{\pi}\int_0^\infty \frac{\lambda}{s^2-\lambda^2}\left(1+\sqrt{\frac{s^2{+}1}{\lambda^2{+}1}}\right)^{-1}\sqrt{\frac{s^2{+}1}{\lambda^2{+}1}}\;\frac{-\lambda}{\lambda^2{+}1}\,ds \\
&=\; \frac{1}{\pi}\frac{1}{\lambda^2{+}1}\int_0^\infty \Big(\sqrt{s^2{+}1}\Big(\sqrt{\lambda^2{+}1}+\sqrt{s^2{+}1}\Big)\Big)^{-1}ds\,.
\end{aligned}$$

By setting $t := s+\sqrt{s^2+1}$, we obtain $\sqrt{s^2+1} = (t^2+1)/(2t)$ and $(t^2+1)\,dt = 2t\,ds$. Hence,

$$\frac{d\vartheta_0}{d\lambda}(\lambda) \;=\; \frac{2}{\pi}\frac{1}{\lambda^2+1}\int_0^\infty \frac{1}{t^2+2\sqrt{\lambda^2+1}\,t+1}\,dt = \frac{1}{\pi}\frac{\tilde{l}_0(\lambda)}{\lambda(\lambda^2+1)}\;, \tag{5.13}$$

where for any $\omega \geqslant 0$,

$$\tilde{l}_\omega(\lambda) \;:=\; \ln\frac{\sqrt{\lambda^2+1+\omega^2}+\sqrt{1+\omega^2}+\lambda}{\sqrt{\lambda^2+1+\omega^2}+\sqrt{1+\omega^2}-\lambda} \;=\; \tilde{l}_0\left(\frac{\lambda}{\sqrt{1+\omega^2}}\right). \tag{5.14}$$

Since (5.13) is positive and differentiable in $\lambda > 0$, ϑ_0 increases monotonically with λ and is twice differentiable. A short calculation shows that

$$\frac{d\tilde{l}_0}{d\lambda}(\lambda) = \frac{1}{\sqrt{\lambda^2+1}} \;<\; 1. \tag{5.15}$$

In particular, since $\tilde{l}_0(0) = 0$, it follows that $\tilde{l}_0(\lambda) \leqslant \lambda$. Thus, (5.13) shows that

$$\frac{d\vartheta_0}{d\lambda}(\lambda) \;\leqslant\; \frac{1}{\pi}\frac{1}{\lambda^2+1}\,, \tag{5.16}$$

which implies the first estimate in (5.11) for any $\omega \geqslant 0$ by using the scaling property.

By differentiating once more, we find

$$\frac{d^2\vartheta_0}{d\lambda^2}(\lambda) \;=\; -\frac{1}{\pi\lambda(\lambda^2+1)^2}\left(\frac{3\lambda^2+1}{\lambda}\,\tilde{l}_0(\lambda) - \sqrt{\lambda^2+1}\right). \tag{5.17}$$

Note that

$$0 \;\leqslant\; \frac{d}{d\lambda}\frac{\lambda}{\sqrt{\lambda^2+1}} \;=\; \frac{1}{\sqrt{\lambda^2+1}} - \frac{\lambda^2}{(\lambda^2+1)^{3/2}} \;\leqslant\; \frac{1}{\sqrt{\lambda^2+1}} \;=\; \frac{d\tilde{l}_0}{d\lambda}(\lambda)\,,$$

which (together with $\tilde{l}_\omega(0) = 0$) implies $\tilde{l}_0(\lambda) \geqslant \lambda/\sqrt{\lambda^2+1}$. In particular, the parenthesis in (5.17) is non-negative for all $\lambda > 0$, and therefore

$$\left|\frac{d^2\vartheta_0}{d\lambda^2}\right| \;=\; \frac{1}{\pi\lambda(\lambda^2+1)^2}\left(\frac{3\lambda^2+1}{\lambda}\,\tilde{l}_0(\lambda) - \sqrt{\lambda^2+1}\right) \;\leqslant\; \frac{3}{\pi}\frac{1}{(\lambda^2+1)^{3/2}}\,, \tag{5.18}$$

where we have used that $\tilde{l}_0(\lambda) \leqslant \lambda$ and $\sqrt{\lambda^2+1}-1 \geqslant 0$ for all $\lambda \geqslant 0$. By the scaling property, this completes the proof of (5.11). Moreover, it follows from

$$\frac{1}{\pi}\frac{1}{(\lambda^2+1)^{3/2}} \;\leqslant\; \frac{d\vartheta_0}{d\lambda} \;\leqslant\; \frac{1}{\pi}\frac{1}{\lambda^2+1}\,,$$

that $\lim_{\lambda\to0^+}\vartheta'_\omega(\lambda) = \frac{1}{\pi}(1+\omega^2)^{-1/2}$.

Next, following [37, Prop. 4.16], by performing the change of variables $t = s/\lambda$ for $0 < s < 1$ and $t = \lambda/s$ for $s > 1$ in (5.9), we find

$$\vartheta_0(\lambda) \;=\; \frac{1}{\pi}\int_0^1 \frac{1}{1-t^2}\;\ln\frac{1+\sqrt{\frac{\lambda^2/t^2+1}{\lambda^2+1}}}{1+\sqrt{\frac{\lambda^2t^2+1}{\lambda^2+1}}}\;dt\,.$$

By dominated convergence, it follows that $\lim_{\lambda\to0^+}\vartheta_\omega(\lambda) = 0$, and

$$\lim_{\lambda\to\infty}\vartheta_\omega(\lambda) \;=\; \frac{1}{\pi}\int_0^1 \frac{-\ln t}{1-t^2}\,dt \;=\; \frac{\pi}{8}\,.$$

For a proof of the last identity, see for example [37, Prop. 4.15]. □

Let $G_{\omega,\lambda}$ be the second term in the expression (5.3) for $F_{\omega,\lambda}$ and let $\varphi_{\omega,\lambda}$ denote the corresponding function (5.7) in the Laplace transform of $G_{\omega,\lambda}$. The following Lemma provides properties of $\varphi_{\omega,\lambda}$, which will be needed in the proof of Lemma 20 below.

Lemma 19 (Properties of $\varphi_{\omega,\lambda}$)**.** *For all $\lambda > 0$, the function $\varphi_{\omega,\lambda}$ is differentiable in $t = 0$, with*

$$\varphi'_{\omega,\lambda}(0) \;=\; \frac{\lambda^2{+}1{+}\omega^2}{1{+}\omega^2}\,\frac{d\vartheta_\omega}{d\lambda}(\lambda)\,, \tag{5.19}$$

and

$$\lim_{\lambda\to\infty}\varphi'_{\omega,\lambda}(0) \;=\; 0\,, \quad \lim_{\lambda\to 0+}\varphi'_{\omega,\lambda}(0) = \frac{1}{\pi\sqrt{1{+}\omega^2}}\,. \tag{5.20}$$

Proof. If $I_{\lambda,t}(s)$ denotes the integrand in (5.7), then for any $\varepsilon > 0$

$$\frac{1}{\varepsilon}\Big|I_{\lambda,\varepsilon}(s) - I_{\lambda,0}(s)\Big| \;=\; \frac{1}{\varepsilon^2{+}s^2}\ln\frac{1-s^2/\lambda^2}{1-f_\omega(s^2)/f_\omega(\lambda^2)} \;\leqslant\; \frac{1}{s^2}\ln\frac{1-s^2/\lambda^2}{1-f_\omega(s^2)/f_\omega(\lambda^2)} =: h_\lambda(s)\,.$$

We also have

$$\frac{1-s^2/\lambda^2}{1-f_\omega(s^2)/f_\omega(\lambda^2)} = \frac{f_\omega(\lambda^2)}{\lambda^2}\Big(\sqrt{s^2{+}1{+}\omega^2} + \sqrt{\lambda^2{+}1{+}\omega^2}\,\Big)$$

and therefore, by l'Hôpital's rule

$$\lim_{s\to 0+} h_\lambda(s) \;=\; \Big[2\Big(\sqrt{1{+}\omega^2} + \sqrt{\lambda^2{+}1{+}\omega^2}\Big)\sqrt{1{+}\omega^2}\;\Big]^{-1}\,.$$

Hence, h_λ is continuous on $[0,\infty)$ and therefore locally integrable near $s = 0$. Moreover, since $s \mapsto \ln(s)/s^2$ is integrable on $[1,\infty)$, h_λ is an integrable upper bound for the difference quotient above. Thus, by dominated convergence,

$$\frac{d\varphi_{\omega,\lambda}}{dt}(0) \;=\; \frac{1}{\pi}\int_0^\infty \frac{1}{s^2}\,\ln\frac{1-s^2/\lambda^2}{1-f_\omega(s^2)/f_\omega(\lambda^2)}\;ds\,.$$

Hence, by monotone convergence, it follows that

$$\lim_{\lambda\to\infty}\frac{d\varphi_{\omega,\lambda}}{dt}(0) \;=\; \frac{1}{\pi}\int_0^\infty \frac{1}{s^2}\lim_{\lambda\to\infty}\ln\frac{1-s^2/\lambda^2}{1-f_\omega(s^2)/f_\omega(\lambda^2)}\,ds \;=\; 0\,,$$

which proves the first identity in (5.20). Moreover, integrating by parts yields

$$\begin{aligned}\frac{d\varphi_{\omega,\lambda}}{dt}(0) \;&=\; -\frac{1}{\pi}\int_0^\infty\Big(\frac{d}{ds}\frac{1}{s}\Big)\ln\Big[\frac{f_\omega(\lambda^2)}{\lambda^2}\Big(\sqrt{s^2{+}1{+}\omega^2} + \sqrt{\lambda^2{+}1{+}\omega^2}\,\Big)\Big]\\ &=\; \frac{1}{\pi}\int_0^\infty\Big(\sqrt{s^2{+}1{+}\omega^2}\Big(\sqrt{s^2{+}1{+}\omega^2} + \sqrt{\lambda^2{+}1{+}\omega^2}\Big)\Big)^{-1}\,ds \;=\; \frac{\lambda^2{+}1{+}\omega^2}{1{+}\omega^2}\frac{d\vartheta_\omega}{d\lambda}(\lambda)\,,\end{aligned}$$

where the last identity follows by comparing with the calculation leading to (5.13). This shows (5.19), and together with (5.12) also the second identity in (5.20). □

The following result will be used in the proof of Proposition 21 in the next section and also provides a bound on

$$\Lambda^{(2)}_\mu = \int_0^\infty \mathcal{K}_\mu(t)\,dt\,, \tag{5.21}$$

where $\mathcal{K}_\mu$ is defined in (5.23) below.

Lemma 20. *For $0 \leqslant \delta < 1$ there exists $C_\delta > 0$, such that*

$$\int_0^\infty t^\delta |\mathcal{K}_\mu(t)|\, dt \;\leqslant\; C_\delta\, (1+\mu)^{(d-\delta)/2}\,, \tag{5.22}$$

where for $\nu, t > 0$,

$$\mathcal{K}_\mu(t) := \frac{1}{(2\pi)^{d-1}} \int_{\mathbb{R}^{d-1}} |\xi'|^2 \left(\mathcal{J}_{\mu,|\xi'|} - \mathcal{J}^+_{\mu,|\xi'|}(|\xi'|t) \right) d\xi'\,, \tag{5.23}$$

$$\mathcal{J}^+_{\mu,\nu}(t) := \frac{2}{\pi} \int_0^\infty \left(\psi_{\mu/\nu}(\lambda^2{+}1) - \nu^{-1}\right)_- F_{\mu/\nu,\lambda}(t)^2\, d\lambda\,, \tag{5.24}$$

$$\mathcal{J}_{\mu,\nu} := \frac{1}{\pi} \int_0^\infty \left(\psi_{\mu/\nu}(\lambda^2{+}1) - \nu^{-1}\right)_- d\lambda\,. \tag{5.25}$$

Proof. For any $\nu > 0$,

$$\mathcal{J}_{\mu,\nu} - \mathcal{J}^+_{\mu,\nu}(t) \;=\; \pi^{-1} \int_0^\infty \left(\psi_{\mu/\nu}(\lambda^2{+}1) - \nu^{-1}\right)_- \left(1{-}2F_{\mu/\nu,\lambda}(t)^2\right) d\lambda\,,$$

where the integrand can be non-zero only if $\nu^2(1{+}\lambda^2) \leqslant 1{+}2\mu$, i.e. if $0 < \nu \leqslant \sqrt{1{+}2\mu}$ and

$$0 \;<\; \lambda \;\leqslant \left(\frac{1{+}2\mu}{\nu^2} - 1\right)^{1/2}\,. \tag{5.26}$$

By (5.3), we have

$$1 - 2F_{\mu/\nu,\lambda}(t)^2 \;=\; \cos\left(2\beta_{\mu/\nu,t}(\lambda)\right) - 4\sin\left(\beta_{\mu/\nu,t}(\lambda)\right) G_{\mu/\nu,\lambda}(t) - 2G_{\mu/\nu,\lambda}(t)^2\,, \tag{5.27}$$

where $\beta_{\omega,t}(\lambda) := \lambda t + \vartheta_\omega(\lambda)$. Hence, we obtain

$$\int_0^\infty t^\delta \left|\mathcal{J}_{\mu,\nu} - \mathcal{J}^+_{\mu,\nu}(t)\right| dt \;\leqslant\; \pi^{-1} \int_0^\infty t^\delta \Big(|R_1(\nu,t)| + |R_2(\nu,t)|\Big)\, dt \tag{5.28}$$

where

$$R_1(\nu,t) := \int_0^\infty \left(\psi_{\mu/\nu}(\lambda^2{+}1){-}\nu^{-1}\right)_- \cos\left(2\beta_{\mu/\nu,t}(\lambda)\right) d\lambda,$$

$$R_2(\nu,t) := \int_0^\infty \left(\psi_{\mu/\nu}(\lambda^2{+}1){-}\nu^{-1}\right)_- \Big(4\sin\left(\beta_{\mu/\nu,t}(\lambda)\right) G_{\mu/\nu,\lambda}(t) + 2G_{\mu/\nu,\lambda}(t)^2\Big)\, d\lambda.$$

Let $0 < \delta < 1$. We have

$$\cos\left(2\beta_{\mu/\nu,t}(\lambda)\right) \;=\; \frac{1}{2t}\left(\frac{d}{d\lambda}\sin\left(2\beta_{\mu/\nu,t}(\lambda)\right) - 2\cos\left(2\beta_{\mu/\nu,t}(\lambda)\right)\frac{d\vartheta_{\mu/\nu}}{d\lambda}\right)\,, \tag{5.29}$$

and integrating by parts in λ yields

$$\int_0^1 t^\delta\, |R_1(\nu,t)|\, dt \leqslant \int_0^1 \frac{t^{\delta-1}}{2} \int_0^{((1+2\mu)/\nu^2-1)^{1/2}} \left(\left|\frac{d}{d\lambda}\psi_{\mu/\nu}(\lambda^2{+}1)\right| + 2\nu^{-1}\left|\frac{d\vartheta_{\mu/\nu}}{d\lambda}\right| \right) d\lambda\, dt\,.$$

Note that the boundary terms are zero, since by (5.12) we have $\lim_{\lambda\to 0^+} \beta_{\mu/\nu,t}(\lambda) = 0$, and the negative part $(\psi_{\mu/\nu}(\lambda^2{+}1){-}\nu^{-1})_-$ vanishes at $\lambda = ((1{+}2\mu)/\nu^2 - 1)^{1/2}$. We have

$$\frac{d}{d\lambda}\psi_{\mu/\nu}(\lambda^2{+}1) \;=\; \frac{\lambda}{\sqrt{\lambda^2{+}1 + (\mu/\nu)^2}}\,, \tag{5.30}$$

and thus, for any $\Lambda > 0$,

$$\int_0^\Lambda \left|\frac{d}{d\lambda}\psi_{\mu/\nu}(\lambda^2+1)\right| d\lambda = \sqrt{1+(\mu/\nu)^2}\int_0^{\Lambda/\sqrt{1+(\mu/\nu)^2}} \frac{x}{\sqrt{x^2+1}}\,dx$$
$$= \frac{\sqrt{1+(\mu/\nu)^2}}{2}\int_0^{\Lambda^2/(1+(\mu/\nu)^2)} \frac{1}{\sqrt{E+1}}\,dE$$
$$= \sqrt{\Lambda^2+1+(\mu/\nu)^2} - \sqrt{1+(\mu/\nu)^2}$$
$$= \nu^{-1}(1+\mu) - \sqrt{1+(\mu/\nu)^2} < \nu^{-1},$$

where we have substituted $\Lambda = ((1+2\mu)/\nu^2-1)^{1/2}$. Moreover, by (5.11)

$$\int_0^{\sqrt{1+2\mu}/\nu} \left|\frac{d\vartheta_{\mu/\nu}}{d\lambda}\right| d\lambda \leqslant \frac{1}{\pi}\int_0^{\sqrt{1+2\mu}/\nu} \frac{\sqrt{1+(\mu/\nu)^2}}{\lambda^2+1+(\mu/\nu)^2}\,d\lambda \leqslant \frac{1}{\pi}\int_0^\infty \frac{1}{1+x^2}\,dx = \frac{1}{2}.$$

Hence, we obtain

$$\int_0^1 t^\delta\,|R_1(\nu,t)|\,dt \leqslant \delta^{-1}\nu^{-1}. \tag{5.31}$$

In the region $t \in (1,\infty)$, after two integrations by parts, we find

$$\int_1^\infty t^\delta\,|R_1(\nu,t)|\,dt \leqslant \int_1^\infty \frac{t^{\delta-2}}{4}\,dt\left(1+\int_0^{((1+2\mu)/\nu^2-1)^{1/2}}\left(\left|\frac{d^2}{d\lambda^2}\psi_{\mu/\nu}(\lambda^2+1)\right|\right.\right.$$
$$\left.\left.+\,3\left|\frac{d}{d\lambda}\psi_{\mu/\nu}(\lambda^2+1)\right|\left|\frac{d\vartheta_{\mu/\nu}}{d\lambda}\right| + 2\nu^{-1}\left|\frac{d\vartheta_{\mu/\nu}}{d\lambda}\right|^2 + \nu^{-1}\left|\frac{d^2\vartheta_{\mu/\nu}}{d\lambda^2}\right|\right)d\lambda\right),$$

where we used (5.30) to bound the non-zero boundary term. We have

$$\frac{d^2}{d\lambda^2}\psi_{\mu/\nu}(\lambda^2+1) = \frac{1+(\mu/\nu)^2}{\sqrt{\lambda^2+1+(\mu/\nu)^2}^{\,3}} \leqslant \frac{1}{\sqrt{\lambda^2+1+(\mu/\nu)^2}},$$

and thus, for any $\Lambda \geqslant 0$

$$\int_0^\Lambda \left|\frac{d^2}{d\lambda^2}\psi_{\mu/\nu}(\lambda^2+1)\right| d\lambda \leqslant \int_0^{\Lambda/\sqrt{1+(\mu/\nu)^2}} \frac{1}{\sqrt{x^2+1}}\,dx \leqslant \frac{\Lambda}{\sqrt{1+(\mu/\nu)^2}}.$$

Hence in the case $\Lambda = ((1+2\mu)/\nu^2-1)^{1/2}$, the integral is bounded by

$$\frac{\sqrt{1+\mu^2-(\nu^2+\mu^2)}}{\sqrt{\nu^2+\mu^2}} = \sqrt{\frac{1}{\nu^2+\mu^2}+\frac{\mu^2}{\nu^2+\mu^2}-1} \leqslant \frac{1}{\sqrt{\nu^2+\mu^2}}. \tag{5.32}$$

Next, from (5.11) and (5.30), it follows that

$$\int_0^{\sqrt{1+2\mu}/\nu} \left|\frac{d}{d\lambda}\psi_{\mu/\nu}(\lambda^2+1)\right|\left|\frac{d\vartheta_{\mu/\nu}}{d\lambda}\right| d\lambda \leqslant \frac{1}{\pi}\int_0^\infty \frac{1}{x^2+1}\,dx = \frac{1}{2}, \tag{5.33}$$

and

$$\nu^{-1}\int_0^{\sqrt{1+2\mu}/\nu} \left|\frac{d\vartheta_{\mu/\nu}}{d\lambda}\right|^2 d\lambda \leqslant \frac{1}{\pi^2\nu}\int_0^{\sqrt{1+2\mu}/\nu} \frac{1+(\mu/\nu)^2}{(1+(\mu/\nu)^2+\lambda^2)^2}\,d\lambda$$
$$\leqslant \frac{1}{\pi^2\nu}\frac{1}{\sqrt{1+(\mu/\nu)^2}}\int_0^\infty \frac{1}{(x^2+1)^2}\,dx \leqslant \frac{1}{2\pi}\frac{1}{\sqrt{\nu^2+\mu^2}}. \tag{5.34}$$

For the last term, by the second estimate in (5.11), we obtain

$$\nu^{-1}\int_0^{\sqrt{1+2\mu/\nu}}\left|\frac{d^2\vartheta_{\mu/\nu}}{d\lambda^2}\right|d\lambda \;\leqslant\; \frac{3}{\pi\nu}\int_0^{\sqrt{1+2\mu/\nu}}\frac{\sqrt{1+(\mu/\nu)^2}}{(\lambda^2+1+(\mu/\nu)^2)^{3/2}}\,d\lambda$$
$$\leqslant\; \frac{3}{\pi}\frac{1}{\sqrt{\nu^2+\mu^2}}\int_0^\infty\frac{1}{x^2+1}\,dx \;=\; \frac{3}{2}\frac{1}{\sqrt{\nu^2+\mu^2}}\,. \tag{5.35}$$

By combining the estimates (5.32), (5.33), (5.34) and (5.35), we obtain

$$\int_1^\infty t^\delta\,|R_1(\nu,t)|\,dt \;\leqslant\; \frac{1}{1-\delta}\left(1+\frac{1}{\sqrt{\nu^2+\mu^2}}\right).$$

Together with (5.31) this shows that for $0<\delta<1$

$$\int_0^\infty t^\delta|R_1(\nu,t)|\,dt \;\leqslant\; C'_\delta\left(1+\nu^{-1}\right), \tag{5.36}$$

where $C'_\delta = 2\max\{\delta^{-1},(1-\delta)^{-1}\}$.

Next, by Lemma 16, we have $0\leqslant G_{\mu/\nu,\lambda}(t)\leqslant \sin\vartheta_{\mu/\nu}(\lambda)$ for all $t>0$, and therefore

$$\int_0^\infty t^\delta|R_2(\nu,t)|\,dt \;\leqslant\; 6\int_0^{\sqrt{1+2\mu/\nu}}\big(\nu^{-1}-\psi_{\mu/\nu}(\lambda^2+1)\big)\int_0^\infty t^\delta G_{\mu/\nu,\lambda}(t)\,dt\,d\lambda\,. \tag{5.37}$$

By (5.6), for any $\omega>0$

$$\begin{aligned}\int_0^\infty G_{\omega,\lambda}(t)\,dt \;&=\; \frac{\cos\vartheta_\omega(\lambda)}{\lambda}-\sqrt{\frac{f'_\omega(\lambda^2)}{f_\omega(\lambda^2)}}\\ &\leqslant\; \lambda^{-1}-\Big(\lambda^2+\big(\sqrt{\lambda^2+1+\omega^2}-\sqrt{1+\omega^2}\big)^2\Big)^{-1/2}\\ &=\; \frac{\sqrt{\lambda^2+\big(\sqrt{\lambda^2+1+\omega^2}-\sqrt{1+\omega^2}\big)^2}-\lambda}{\lambda\sqrt{\lambda^2+\big(\sqrt{\lambda^2+1+\omega^2}-\sqrt{1+\omega^2}\big)^2}}\,.\end{aligned}$$

From here we can perform two different estimates which will be suitable in the cases $\lambda\leqslant 1$ and $\lambda>1$ respectively. By using

$$\sqrt{x^2+c^2}-c\;\leqslant\;\frac{x^2}{2c}\,,\qquad \sqrt{x^2+c^2}-c\;\leqslant\;x\,,\qquad \forall x,c>0\,, \tag{5.38}$$

we find

$$\frac{\sqrt{\lambda^2+\big(\sqrt{\lambda^2+1+\omega^2}-\sqrt{1+\omega^2}\big)^2}-\lambda}{\lambda\sqrt{\lambda^2+\big(\sqrt{\lambda^2+1+\omega^2}-\sqrt{1+\omega^2}\big)^2}} \;\leqslant\; \frac{\big(\sqrt{\lambda^2+1+\omega^2}-\sqrt{1+\omega^2}\big)^2}{2\lambda^2\sqrt{\lambda^2+\big(\sqrt{\lambda^2+1+\omega^2}-\sqrt{1+\omega^2}\big)^2}} \leqslant \frac{\lambda}{8(1+\omega^2)}$$

and on the other hand

$$\frac{\sqrt{\lambda^2+\big(\sqrt{\lambda^2+1+\omega^2}-\sqrt{1+\omega^2}\big)^2}-\lambda}{\lambda\sqrt{\lambda^2+\big(\sqrt{\lambda^2+1+\omega^2}-\sqrt{1+\omega^2}\big)^2}} \;\leqslant\; \frac{\sqrt{\lambda^2+1+\omega^2}-\sqrt{1+\omega^2}}{\lambda\sqrt{\lambda^2+\big(\sqrt{\lambda^2+1+\omega^2}-\sqrt{1+\omega^2}\big)^2}} \;\leqslant\; \frac{1}{\lambda}\,.$$

Hence, we obtain for all $\omega,\lambda>0$

$$\int_0^\infty G_{\omega,\lambda}(t)\,dt \;\leqslant\; \min\{\lambda,\lambda^{-1}\}\,. \tag{5.39}$$

By differentiating (5.6), we also get that for any $\omega, \lambda > 0$

$$\begin{aligned}\int_0^\infty t G_{\omega,\lambda}(t)\, dt &= \varphi'_{\omega,\lambda}(0) \sqrt{\frac{f'_\omega(\lambda^2)}{f_\omega(\lambda^2)}} - \frac{\sin \vartheta_\omega(\lambda)}{\lambda^2} \\ &= \frac{\lambda^2{+}1{+}\omega^2}{1{+}\omega^2} \frac{d\vartheta_\omega}{d\lambda}(\lambda) \sqrt{\frac{f'_\omega(\lambda^2)}{f_\omega(\lambda^2)}} - \frac{\sin \vartheta_\omega(\lambda)}{\lambda^2} \\ &\overset{(5.13)}{=} \frac{1}{\lambda} \left(\frac{\tilde{l}_\omega(\lambda)}{\pi} \sqrt{\frac{f'_\omega(\lambda^2)}{f_\omega(\lambda^2)}} - \frac{\sin(\vartheta_\omega(\lambda))}{\lambda} \right), \end{aligned} \tag{5.40}$$

where $\tilde{l}_\omega$ denotes the logarithm (5.14). By Taylor's theorem, there exists $r_\omega \in \mathcal{O}(1)$ as $\lambda \to 0+$, such that

$$\sin(\vartheta_\omega(\lambda)) = \cos(\vartheta_\omega(0+))\, \vartheta'_\omega(0+)\, \lambda + \lambda^2\, r_\omega(\lambda) = \frac{\lambda}{\pi\sqrt{1{+}\omega^2}} + \lambda^2\, r_\omega(\lambda)\,, \tag{5.41}$$

since $\vartheta''_\omega(0+) = 0$ by Lemma 18. Hence it follows that

$$\int_0^\infty t G_{\omega,\lambda}(t)\, dt \leqslant \frac{1}{\pi\lambda} \left| \tilde{l}_\omega(\lambda) \sqrt{\frac{f'_\omega(\lambda^2)}{f_\omega(\lambda^2)}} - \frac{1}{\sqrt{1{+}\omega^2}} \right| + |r_\omega(\lambda)|\,. \tag{5.42}$$

Note that, by using the Lagrange form of the remainder, for each $\lambda > 0$ we can find $\zeta \in (0, \lambda)$ such that

$$\begin{aligned}|r_\omega(\lambda)| &= \frac{1}{2} \left| \vartheta'_\omega(\zeta)^2 \sin \vartheta_\omega(\zeta) + \vartheta''_\omega(\zeta) \cos \vartheta_\omega(\zeta) \right| \\ &\leqslant \frac{1}{\pi} \frac{1{+}\omega^2}{(\zeta^2{+}1{+}\omega^2)^2} + \frac{3}{2\pi} \frac{\zeta\sqrt{1{+}\omega^2}}{(\zeta^2{+}1{+}\omega^2)^{3/2}} \\ &\leqslant \frac{1}{\pi} \frac{1}{\zeta^2{+}1{+}\omega^2} + \frac{3}{2\pi} \frac{1}{\sqrt{\zeta^2{+}1{+}\omega^2}} \leqslant \frac{5}{2\pi} \frac{1}{\sqrt{\zeta^2{+}1{+}\omega^2}}\,, \end{aligned} \tag{5.43}$$

in particular $|r_\omega(\lambda)| < (1{+}\omega^2)^{-1/2}$ for all $\omega, \lambda > 0$.

We proceed by studying (5.42) first for small λ, more precisely for $\lambda < (1{+}\omega^2)^{-1/2}$. Since

$$\sqrt{\frac{f_\omega(\lambda^2)}{f'_\omega(\lambda^2)}} = \sqrt{\lambda^2 + \left(\sqrt{\lambda^2{+}1{+}\omega^2} - \sqrt{1{+}\omega^2} \right)^2} \leqslant \lambda\sqrt{1{+}\lambda^2}\,,$$

we have for $0 < \lambda \leqslant (1{+}\omega^2)^{-1/2}$, that

$$\left(\frac{1}{\sqrt{1{+}\omega^2}} - \lambda \right) \sqrt{\frac{f_\omega(\lambda^2)}{f'_\omega(\lambda^2)}} \leqslant \frac{1{-}\lambda}{\sqrt{1{+}\omega^2}} \sqrt{\frac{f_\omega(\lambda^2)}{f'_\omega(\lambda^2)}} \leqslant \frac{\lambda(1{-}\lambda)\sqrt{1{+}\lambda^2}}{\sqrt{1{+}\omega^2}}\,. \tag{5.44}$$

Furthermore,

$$\frac{d}{d\lambda} \lambda(1{-}\lambda)\sqrt{1{+}\lambda^2} = (1{-}2\lambda)\sqrt{1{+}\lambda^2} + (1{-}\lambda) \frac{\lambda^2}{\sqrt{1{+}\lambda^2}} \leqslant (1{-}\lambda)(1{+}2\lambda^2)\,. \tag{5.45}$$

The basic estimates

$$\sqrt{\lambda^2{+}1{+}\omega^2} - \sqrt{1{+}\omega^2} \leqslant \frac{\lambda^2}{2} \leqslant \lambda(\lambda^2 + (1{-}\lambda)^2) \leqslant \sqrt{\lambda^2{+}1{+}\omega^2} \left(\lambda(1{+}2\lambda^2) - 2\lambda^2 \right)$$

imply

$$(1{+}2\lambda^2)\sqrt{\lambda^2{+}1{+}\omega^2} \leqslant \sqrt{1{+}\omega^2} + \lambda(1{+}2\lambda^2)\sqrt{\lambda^2{+}1{+}\omega^2}\,,$$

and therefore

$$(1-\lambda)(1+2\lambda^2)\sqrt{\lambda^2+1+\omega^2} \leqslant \sqrt{1+\omega^2}\,.$$

Hence, by (5.45)

$$\frac{d}{d\lambda}\frac{\lambda(1-\lambda)\sqrt{1+\lambda^2}}{\sqrt{1+\omega^2}} \leqslant \frac{1}{\sqrt{\lambda^2+1+\omega^2}} \overset{(5.15)}{=} \frac{d}{d\lambda}\tilde{l}_\omega(\lambda)\,,$$

which implies

$$\tilde{l}_\omega(\lambda) \;\geqslant\; \frac{\lambda(1-\lambda)\sqrt{1+\lambda^2}}{\sqrt{1+\omega^2}} \overset{(5.44)}{\geqslant} \left(\frac{1}{\sqrt{1+\omega^2}}-\lambda\right)\sqrt{\frac{f_\omega(\lambda^2)}{f'_\omega(\lambda^2)}}\,, \tag{5.46}$$

since $\tilde{l}_\omega(0) = 0$.

Furthermore, in the proof of Lemma 18, we have shown that $\tilde{l}_\omega(\lambda) \leqslant \lambda/\sqrt{1+\omega^2}$ for all $\lambda > 0$. Thus

$$\tilde{l}_\omega(\lambda)\sqrt{\frac{f'_\omega(\lambda^2)}{f_\omega(\lambda^2)}} \;\leqslant\; \frac{1}{\sqrt{1+\omega^2}}\frac{\lambda}{\sqrt{\lambda^2+\left(\sqrt{\lambda^2+1+\omega^2}-\sqrt{1+\omega^2}\right)^2}} \leqslant \frac{1}{\sqrt{1+\omega^2}}\,, \tag{5.47}$$

and therefore, by (5.42),

$$\int_0^\infty t\,G_{\omega,\lambda}(t)\,dt \;\leqslant\; \frac{1}{\pi\lambda}\left(\frac{1}{\sqrt{1+\omega^2}} - \tilde{l}_\omega(\lambda)\sqrt{\frac{f'_\omega(\lambda^2)}{f_\omega(\lambda^2)}}\right) + |r_\omega(\lambda)|\,.$$

Together with (5.46) and (5.43), in the case of $0 < \lambda \leqslant (1+\omega^2)^{-1/2}$, it follows that

$$\int_0^\infty t\,G_{\omega,\lambda}(t)\,dt \;\leqslant\; \frac{1}{\pi} + |r_\omega(\lambda)| \;\leqslant\; \frac{7}{2\pi}\,.$$

Next, for $(1+\omega^2)^{-1/2} < \lambda \leqslant 1$, we obtain from (5.42), (5.43) and (5.47) that

$$\int_0^\infty t\,G_{\omega,\lambda}(t)\,dt \;\leqslant\; \frac{2}{\pi\lambda}\frac{1}{\sqrt{1+\omega^2}} + \frac{5}{2\pi}\frac{1}{\sqrt{1+\omega^2}} \;<\; \frac{9}{2\pi}\,.$$

And finally, for $\lambda > 1$, by using (5.40) and (5.47) we obtain

$$\int_0^\infty tG_{\omega,\lambda}(t)\,dt \;\leqslant\; \frac{1}{\lambda}\left(\frac{1}{\pi\sqrt{1+\omega^2}} + \frac{1}{\lambda}\right) \;<\; \frac{2}{\lambda}\,.$$

Hence, for any $\lambda > 0$, we have

$$\int_0^\infty t\,G_{\omega,\lambda}(t)\,dt \;<\; 2\min\{1,\lambda^{-1}\}\,. \tag{5.48}$$

Combining (5.39) and (5.48) it follows for all $0 \leqslant \delta < 1$, that

$$\int_0^\infty t^\delta G_{\mu/\nu,\lambda}(t)\,dt \;\leqslant\; \int_0^1 G_{\mu/\nu,\lambda}(t)\,dt + \int_1^\infty t\,G_{\mu/\nu,\lambda}(t)\,dt \;<\; 3\min\{1,\lambda^{-1}\}\,.$$

Thus, by (5.37)

$$\int_0^\infty t^\delta|R_2(\nu,t)|\,dt \;\leqslant\; 18\nu^{-1}\int_0^{\sqrt{1+2\mu}/\nu}\min\{1,\lambda^{-1}\}\,d\lambda \;=\; 18\,\nu^{-1}\left(1+\ln\frac{\sqrt{1+2\mu}}{\nu}\right).$$

Together with (5.36), (5.28) implies for $0 < \delta < 1$ that

$$\int_0^\infty t^\delta\left|\mathcal{J}_{\mu,\nu} - \mathcal{J}^+_{\mu,\nu}(t)\right|\,dt \;\leqslant\; C_\delta\left(1+\nu^{-1}+\nu^{-1}\ln\frac{\sqrt{1+2\mu}}{\nu}\right), \tag{5.49}$$

and therefore

$$\begin{aligned}\int_0^\infty t^\delta |\mathcal{K}_\mu(t)|\,dt &= \frac{1}{(2\pi)^{d-1}}\int_{\mathbb{R}^{d-1}} |\xi'|^2 \int_0^\infty t^\delta \left|\mathcal{J}_{\mu,|\xi'|} - \mathcal{J}^+_{\mu,|\xi'|}(|\xi'|t)\right| dt\,d\xi' \\ &= \frac{|\mathbb{S}^{d-2}|}{(2\pi)^{d-1}} \int_0^{\sqrt{1+2\mu}} \nu^{d-1-\delta} \int_0^\infty s^\delta \left|\mathcal{J}_{\mu,\nu} - \mathcal{J}^+_{\mu,\nu}(s)\right| ds\,d\nu \\ &\leqslant C_\delta\,(1+2\mu)^{(d-\delta)/2}\left(\int_0^1 r^{d-1-\delta}dr + \int_0^1 r^{d-2-\delta}(1-\ln r)dr\right).\end{aligned}$$

Since $\int_0^1 r^{-\beta}dr < \infty$ and $|\int_0^1 r^{-\beta}\ln r\,dr| < \infty$ for any $\beta < 1$, it follows that

$$\int_0^\infty t^\delta |\mathcal{K}_\mu(t)|\,dt \leqslant C_\delta\,(1+\mu)^{(d-\delta)/2}$$

for some constant $C_\delta > 0$ depending only on $\delta \in (0,1)$ and $d \geqslant 2$.

In the case $\delta = 0$, the above calculation can be done in the same way except for the integration of $|R_1(\nu,t)|$ for small t. Here we have

$$\int_0^\nu |R_1(\nu,t)|\,dt \leqslant \frac{\sqrt{1+2\mu}}{\nu},$$

whereas in the region $\nu \leqslant t \leqslant \sqrt{1+2\mu}$ integration by parts in λ yields

$$\int_\nu^{\sqrt{1+2\mu}} |R_1(\nu,t)|\,dt \leqslant \nu^{-1}\int_\nu^1 t^{-1}\,dt = \nu^{-1}\ln\frac{\sqrt{1+2\mu}}{\nu},$$

just as in the calculation leading to (5.31). Hence we obtain the same terms as above, and so the claim also follows for $\delta = 0$. □

6. Analysis on the half-space

In this section, as an application of the results from Sections 4 and 5, we prove

Proposition 21. *For all $\delta_1, \delta_2 \in (0,1)$ there exist constants $C_{\delta_1}, C_{\delta_1,\delta_2} > 0$ such that for all real-valued $\phi \in C_0^1(\mathbb{R}^d)$ supported in a ball of radius 1,*

$$\begin{aligned}&- C_{\delta_1,\delta_2}\left((1+\mu)^{(d-\delta_2)/2}h^{-d+1+\delta_2} + (1+\mu)^{(d-\delta_1)/2}h^{-d+1+\delta_1}\right) \\ &\leqslant \operatorname{Tr}\left(\phi H^+_{\mu,h}\phi\right)_- - h^{-d}\Lambda^{(1)}_\mu \int_{\mathbb{R}^d_+}\phi(x)^2dx + h^{-d+1}\Lambda^{(2)}_\mu\int_{\mathbb{R}^{d-1}}\phi(x',0)^2\,dx' \\ &\leqslant C_{\delta_1}\,(1+\mu)^{(d-\delta_1)/2}\,h^{-d+1+\delta_1}, \end{aligned} \tag{6.1}$$

where $\Lambda^{(2)}_\mu = \int_0^\infty \mathcal{K}_\mu(t)\,dt$, with $\mathcal{K}_\mu$ given by (5.23) above.

This is the analogue of [24, Proposition 8] for $\mu > 0$. The main ingredient for its proof is the following spectral representation of $hA^+_{\mu/h}$, which follows directly from the main results of Sections 4 and 5.

Lemma 22 (Diagonalization)**.** *The operator*

$$V_h : L^2(\mathbb{R}^d_+) \to L^2(\mathbb{R}^d_+),\ (V_hf)(\xi',\xi_d) := \left[\Pi_{\mu/|\xi'|}(U_hf)_{\xi'}\right](\xi_d)$$

which, for any $f \in L^1 \cap L^2(\mathbb{R}^d_+)$, is explicitly given by

$$V_h f(\xi) = \int_{\mathbb{R}^d_+} v_h(\xi, x) f(x)\, dx \qquad \forall \xi = (\xi', \xi_d) \in \mathbb{R}^d_+\,,$$

where $v_h(\xi, x) := h^{-d/2} v(\xi, h^{-1}x)$ and

$$v(\xi, x) := |\xi'|^{1/2} \frac{e^{-i\xi' x'}}{(2\pi)^{(d-1)/2}} \sqrt{\frac{2}{\pi}}\, F_{\mu/|\xi'|,\xi_d}(|\xi'| x_d)\,, \tag{6.2}$$

is unitary and establishes the unitary equivalence of $hA^+_{\mu/h}$ with the operator of multiplication by $a_\mu(\xi', \xi_d) := |\xi'|\psi_{\mu/|\xi'|}(\xi_d^2{+}1)$, i.e.

$$V_h h A^+_{\mu/h} V_h^* = a_\mu\,. \tag{6.3}$$

Proof. Proposition 15 (Section 4) together with Corollary 17 (Section 5). □

Using this, we derive the following representation of $\operatorname{Tr} \phi(H^+_{\mu,h})_- \phi$, which will be used to prove the lower bound in Proposition 21.

Lemma 23. *For any real-valued $\phi \in C^1_0(\mathbb{R}^d)$ we have*

$$\operatorname{Tr} \phi\big(H^+_{\mu,h}\big)_- \phi \;=\; \int_{\mathbb{R}^d_+} \int_{\mathbb{R}^d_+} |\xi'| \big(a_\mu(\xi){-}1\big)_- |v_h(\xi, x)|^2\, d\xi\, \phi(x)^2\, dx \tag{6.4}$$

$$=\; h^{-d}\, \Lambda^{(1)}_\mu \int_{\mathbb{R}^d_+} \phi(x)^2 dx - h^{-d+1} \int_{\mathbb{R}^d_+} \phi(x)^2 h^{-1} \mathcal{K}_\mu(h^{-1}x_d)\, dx\,, \tag{6.5}$$

where $\mathcal{K}_\mu$ was defined in (5.23).

Proof. Since, by the definitions of $a_\mu(\xi)$, $v_h(\xi, x)$ and $\mathcal{J}^+_{\mu,|\xi'|}(t)$,

$$\int_{\mathbb{R}^d_+} |\xi'| \big(a_\mu(\xi){-}1\big)_- |v_h(\xi, x)|^2\, d\xi = \frac{h^{-d}}{(2\pi)^{d-1}} \int_{\mathbb{R}^{d-1}} |\xi'|^2\, \mathcal{J}^+_{\mu,|\xi'|}(h^{-1}|\xi'| x_d)\, d\xi'\,,$$

and, by changing variables,

$$\frac{1}{(2\pi)^{d-1}} \int_{\mathbb{R}^d_+} \int_{\mathbb{R}^{d-1}} |\xi'|^2\, \mathcal{J}_{\mu,|\xi'|}\, d\xi'\, \phi(x)^2\, dx \;=\; \Lambda^{(1)}_\mu \int_{\mathbb{R}^d_+} \phi(x)^2\, dx\,,$$

it follows from the definition of $\mathcal{K}_\mu$, i.e.

$$\mathcal{K}_\mu(t) \;=\; \frac{1}{(2\pi)^{d-1}} \int_{\mathbb{R}^{d-1}} |\xi'|^2 \Big(\mathcal{J}_{\mu,|\xi'|} - \mathcal{J}^+_{\mu,|\xi'|}(|\xi'| t)\Big)\, d\xi'\,,$$

that (6.5) is a direct consequence of (6.4).

For simplicity we write $a := a_\mu$ and $V := V_h$. First, we will show that $(a{-}1)^0_- V\phi V^*$ and $(a{-}1)_- V\phi V^*$ are Hilbert-Schmidt operators. For any $0 \leqslant \delta \leqslant 1$ we have

$$\int_{\mathbb{R}^d_+} \big(a(\xi){-}1\big)^\delta_- \int_{\mathbb{R}^d_+} |V\phi V^*(\xi, \zeta)|^2 d\zeta\, d\xi \tag{6.6}$$

$$= \int_{\mathbb{R}^d_+} \big(a(\xi){-}1\big)^\delta_- \int_{\mathbb{R}^d_+} \left| \int_{\mathbb{R}^d_+} v_h(\xi, x)\phi(x)\overline{v_h(\zeta, x)}\, dx \right|^2 d\zeta\, d\xi$$

$$= \lim_{c\to 0^+} \lim_{b\to 0^+} \int_{\mathbb{R}^d_+} \big(a(\xi){-}1\big)^\delta_- \int_{\mathbb{R}^d_+} e^{-c|\xi'-\zeta'|^2} e^{-b f_{\mu/|\xi'|}(\zeta_d^2)} \left| \int_{\mathbb{R}^d_+} v_h(\xi, x)\phi(x)\overline{v_h(\zeta, x)}\, dx \right|^2 d\zeta\, d\xi\,,$$

where $f_w(t) = \psi_w(t{+}1) - \psi_w(1)$ for any $w \geqslant 0$ (see (5.10)). Note that if $(P_{\omega,b})_{b\geqslant 0}$ denotes the contraction semigroup generated by $-T_\omega^+{+}\psi_\omega(1)$ (see Corollary 17), then by Lemma 16

$$P_{\omega,b}\, g(t) = \big(\Pi_\omega^* e^{-bf_\omega(|\cdot|^2)}\Pi_\omega g\big)(t) = \frac{2}{\pi}\int_0^\infty\int_0^\infty F_{\omega,\lambda}(t)F_{\omega,\lambda}(s)e^{-bf_\omega(\lambda^2)}g(s)\,ds\,d\lambda$$

for all $g \in L^1(0,\infty)\cap L^2(\mathbb{R}_+)$. Hence, if $k_{\omega,b}(t,s) := \frac{2}{\pi}\int_0^\infty F_{\omega,\lambda}(t)F_{\omega,\lambda}(s)e^{-bf_\omega(\lambda^2)}d\lambda$ then

$$\int_0^\infty k_{\omega,b}(\cdot,s)g(s)\,ds \ \xrightarrow{\|\cdot\|_2}\ g$$

as $b\to 0^+$, since $(P_{\omega,b})_{b\geqslant 0}$ is strongly continuous and $P_{\omega,0} = \mathbb{I}$. In particular, by changing variables we obtain for any $\beta > 0$ that

$$\beta\int_0^\infty\int_0^\infty \overline{f(t)}\,k_{\omega,b}(\beta t,\beta s)\,g(s)\,ds\,dt \ \xrightarrow{b\to 0^+}\ (f,g)_{L^2(\mathbb{R}_+)} \tag{6.7}$$

for all $f,g \in L^1(0,\infty)\cap L^2(\mathbb{R}_+)$. And similarly, from $\|P_{w,b}g\|_2 \leqslant \|g\|_2$ we obtain the uniform bound

$$\left|\beta\int_0^\infty\int_0^\infty \overline{f(t)}\,k_{\omega,b}(\beta t,\beta s)\,g(s)\,ds\,dt\right| \ \leqslant\ \|f\|_2\,\|g\|_2\,,$$

which allows the use of dominated convergence in the calculation below. We have

$$\begin{aligned}
&\int_{\mathbb{R}^d_+}\big(a(\xi){-}1\big)_-^\delta\int_{\mathbb{R}^d_+} e^{-c|\xi'-\zeta'|^2}e^{-bf_{\mu/|\xi'|}(\zeta_d^2)}\left|\int_{\mathbb{R}^d_+} v_h(\xi,x)\phi(x)\overline{v_h(\zeta,x)}\,dx\right|^2 d\zeta\,d\xi\\
&= \frac{2}{\pi}\frac{h^{-2d}}{(2\pi)^{2(d-1)}}\int_{\mathbb{R}^d_+}\big(a(\xi){-}1\big)_-^\delta|\xi'|\int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+} F_{\mu/|\xi'|,\xi_d}\big(h^{-1}|\xi'|x_d\big)F_{\mu/|\xi'|,\xi_d}\big(h^{-1}|\xi'|y_d\big)\,\phi(x)\phi(y)\\
&\quad\times\int_{\mathbb{R}^{d-1}} e^{-i(\xi'-\zeta')(x'-y')/h}e^{-c|\xi'-\zeta'|^2}\,|\zeta'|\,k_{\mu/|\zeta'|,b}\big(h^{-1}|\zeta'|x_d, h^{-1}|\zeta'|y_d\big)\,d\zeta'\,dy\,dx\,d\xi\\
&= \frac{2}{\pi}\frac{h^{-2d+1}}{(2\pi)^{2(d-1)}}\int_{\mathbb{R}^d_+}\big(a(\xi){-}1\big)_-^\delta|\xi'|\int_{\mathbb{R}^{d-1}}\int_{\mathbb{R}^{d-1}}\int_{\mathbb{R}^{d-1}} e^{-i(\xi'-\zeta')(x'-y')/h}e^{-c|\xi'-\zeta'|^2}\\
&\quad\times\int_0^\infty\int_0^\infty h^{-1}|\zeta'|\,g_{\xi,x'}(x_d)\,k_{\mu/|\zeta'|,b}\big(h^{-1}|\zeta'|x_d, h^{-1}|\zeta'|y_d\big)g_{\xi,y'}(y_d)\,dy_d\,dx_d\,d\zeta'\,dy'\,dx'\,d\xi\,,
\end{aligned}$$

where $g_{\xi,x'}(x_d) := F_{\mu/|\xi'|,\xi_d}\big(h^{-1}|\xi'|x_d\big)\,\phi(x)$. By (6.6), (6.7) and dominated convergence, we obtain that

$$\int_{\mathbb{R}^d_+}\big(a(\xi){-}1\big)_-^\delta\int_{\mathbb{R}^d_+}|V\phi V^*(\xi,\zeta)|^2 d\zeta\,d\xi \ =\ \frac{h^{-d}}{(2\pi)^{d-1}}\frac{2}{\pi}\lim_{c\to 0^+} I_c\,,$$

where

$$\begin{aligned}
I_c \ :=\ &\frac{1}{(2\pi h)^{d-1}}\int_{\mathbb{R}^d_+}\big(a(\xi){-}1\big)_-^\delta|\xi'|\int_{\mathbb{R}^{d-1}}\int_{\mathbb{R}^{d-1}}\int_{\mathbb{R}^{d-1}} e^{-i(\xi'-\zeta')(x'-y')/h}e^{-c|\xi'-\zeta'|^2}d\zeta'\\
&\quad\times\int_0^\infty F_{\mu/|\xi'|,\xi_d}\big(h^{-1}|\xi'|x_d\big)^2\,\phi(x',x_d)\,\phi(y',x_d)\,dx_d\,dy'\,dx'\,d\xi\\
=\ &\int_{\mathbb{R}^d_+}\phi(x)\int_{\mathbb{R}^d_+}\big(a(\xi){-}1\big)_-^\delta|\xi'|\,F_{\mu/|\xi'|,\xi_d}\big(h^{-1}|\xi'|x_d\big)^2 d\xi\int_{\mathbb{R}^{d-1}}\beta_c(x'{-}y')\phi(y',x_d)\,dy'\,dx\,,
\end{aligned}$$

since we have $(2\pi h)^{-(d-1)}(\mathcal{F}e^{-c|\cdot|^2})(\frac{x'-y'}{2\pi h}) = \beta_c^{(d-1)}(x'-y')$. Here $(\beta_c^{(d-1)})_{c\geqslant 0}$ is the approximate identity given in (2.7) (see Appendix D.1). Hence,

$$\lim_{c\to 0^+} I_c = \int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+} \big(a(\xi)-1\big)_-^\delta |\xi'|\, F_{\mu/|\xi'|,\xi_d}\big(h^{-1}|\xi'|x_d\big)^2 d\xi\, \phi(x)^2\, dx\,. \tag{6.8}$$

In particular, since $\xi\mapsto|\xi'|(a(\xi)-1)_-^\delta$ belongs to $L^1(\mathbb{R}^d_+)$ for any $0\leqslant\delta\leqslant 1$ and $d\geqslant 2$,

$$\int_{\mathbb{R}^d_+} \big(a(\xi)-1\big)_-^\delta \int_{\mathbb{R}^d_+} |V\phi V^*(\xi,\zeta)|^2 d\zeta\, d\xi \,<\, \infty\,, \tag{6.9}$$

and thus $(a-1)_-^0 V\phi V^*$ and $(a-1)_- V\phi V^*$ are Hilbert-Schmidt operators. It follows that

$$\operatorname{Tr}\phi\big(hA^+_{\mu/h}-1\big)_-\phi \,=\, \operatorname{Tr} V\phi V^*(a-1)_- V\phi V^* \,=\, \int_{\mathbb{R}^d_+}\big(a(\xi)-1\big)_- \int_{\mathbb{R}^d_+} |V\phi V^*(\xi,\zeta)|^2 d\zeta\, d\xi\,.$$

Hence, (6.4) follows from (6.8) with $\delta=1$. □

For the upper bound in Proposition 21 we use

Lemma 24. *Let $\phi\in C_0^1(\mathbb{R}^d)$ be real-valued and let $\rho:=\chi(H^+_{\mu,h})_-^0\chi$, where χ denotes the characteristic function of $\operatorname{supp}(\phi)\cap\mathbb{R}^d_+$. Then ρ has range in the form domain of $\phi H^+_{\mu,h}\phi$, and*

$$\operatorname{Tr}\rho\phi H^+_{\mu,h}\phi \,=\, -h^{-d}\Lambda^{(1)}_\mu \int_{\mathbb{R}^d_+}\phi(x)^2\,dx \,+\, h^{-d+1}\int_{\mathbb{R}^d_+}\phi(x)^2 h^{-1}\mathcal{K}_\mu(h^{-1}x_d)\,dx \,-\, R_{\mu,h}(\phi)\,,$$

where for any $\sigma\in(0,\frac12)$,

$$|R_{\mu,h}(\phi)| \,\leqslant\, C_\sigma\,(1+\mu)^{(d-2\sigma)/2}\, h^{-d+1+2\sigma}\,. \tag{6.10}$$

Proof. Since by definition $\rho f=0$ in the complement of $\mathbb{R}^d_+$, similarly as in the proof of Proposition 8, it follows that ρf belongs to the form domain of $\phi A^+_{\mu/h}\phi$ for all $f\in L^2(\mathbb{R}^d)$. Moreover,

$$\begin{aligned}
&\operatorname{Tr}\rho\phi H^+_{\mu,h}\phi \,=\, \operatorname{Tr}\rho\phi hA^+_{\mu/h}\phi - \operatorname{Tr}\rho\phi^2\\
&= \int_{\mathbb{R}^d_+}\big(a_\mu(\xi)-1\big)_-^0\Big[\big(\phi^+\overline{v_h(\xi,\cdot)}, hA^+_{\mu/h}\phi^+\overline{v_h(\xi,\cdot)}\big) - \int_{\mathbb{R}^d_+}|v_h(\xi,x)|^2\,\phi(x)^2\,dx\Big]\,d\xi\,,
\end{aligned} \tag{6.11}$$

where $\phi^+:=\chi\phi$. For $\varphi\in H_0^1(\mathbb{R}^d_+)$, by the integral representation (E.28), we have

$$\begin{aligned}
(\varphi, A^+_{\mu/h}\varphi) &= \lim_{\delta\to0^+}(\varphi, A^+_{\mu/h}e^{-\delta A^+_{\mu/h}}\varphi) = -\lim_{\delta\to0^+}\frac{d}{d\varepsilon}\Big|_{\varepsilon=\delta}\big(\varphi, e^{-\varepsilon A^+_{\mu/h}}\varphi\big)\\
&= \lim_{\delta,\varepsilon\to0^+}\frac{1}{\varepsilon}\Big[(\varphi, e^{-\delta A^+_{\mu/h}}\varphi)-(\varphi, e^{-(\delta+\varepsilon)A^+_{\mu/h}}\varphi)\Big]\\
&= \lim_{\delta,\varepsilon\to0^+}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\big|\varphi(x)-\varphi(y)\big|^2\,\theta^{\delta,\varepsilon}_{\mu/h}(|x-y|)\,dx\,dy\,,
\end{aligned}$$

where for $\nu>0$, $\theta_\nu(t):=\nu^{d+1}\theta(\nu t)$ with $\theta(t):=(2\pi t)^{-(d+1)/2}K_{(d+1)/2}(t)$, and for $\nu,\delta,\varepsilon>0$

$$\theta^{\delta,\varepsilon}_\nu := \frac{1}{\varepsilon}\Big((\delta+\varepsilon)\,\theta^{\delta+\varepsilon}_\nu - \delta\,\theta^\delta_\nu\Big)\,,\quad \theta^\delta_\nu(t) \,:=\, \theta_\nu\big((t^2+\delta^2)^{1/2}\big)\,,$$

in particular $\theta_\nu^0 = \theta_\nu$. Also, we write $\lim_{\delta,\varepsilon\to 0^+}$ to denote the consecutive limits $\lim_{\delta\to 0^+}\lim_{\varepsilon\to 0^+}$, while keeping track of the order of limits. Hence, we have

$$\begin{aligned}
&\Big(\phi^+\overline{v_h(\xi,\cdot)}, A^+_{\mu/h}\phi^+\overline{v_h(\xi,\cdot)}\Big)\\
&= \lim_{\delta,\varepsilon\to 0^+}\int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+}\big|\phi(x)\overline{v_h(\xi,h)} - \phi(y)\overline{v_h(\xi,y)}\big|^2\theta^{\delta,\varepsilon}_{\mu/h}(|x-y|)\,dx\,dy\\
&= \lim_{\delta,\varepsilon,\beta\to 0^+}\int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+}\big|\phi(x)\overline{v_h(\xi,x)} - \phi(y)\overline{v_h(\xi,y)}\big|^2 e_\beta(x)e_\beta(y)\,\theta^{\delta,\varepsilon}_{\mu/h}(|x-y|)\,dx\,dy\,,
\end{aligned}$$

where $e_\beta(x) := e^{-\beta_1|x'|^2}e^{-\beta_2 x_d}$ and $\beta = (\beta_1,\beta_2)\in\mathbb{R}^2_+$. For fixed $h>0$ and $\xi\in\mathbb{R}^d_+$, using $v := v_h(\xi,\cdot)$ as a temporary notation, we write for all $x,y\in\mathbb{R}^d_+$

$$\begin{aligned}
\big|\phi(x)\overline{v_h(\xi,x)} - \phi(y)\overline{v_h(\xi,y)}\big|^2 \;&=\; \frac12\Big(v(x)\overline{v(y)}(\phi(x)-\phi(y))^2 + \overline{v(x)}v(y)(\phi(x)-\phi(y))^2\Big)\\
&\quad + \frac12\phi(x)^2\big(2|v(x)|^2 - v(x)\overline{v(y)} - \overline{v(x)}v(y)\big)\\
&\quad + \frac12\phi(y)^2\big(2|v(y)|^2 - v(y)\overline{v(x)} - \overline{v(y)}v(x)\big)\,,
\end{aligned}$$

so that

$$\big(\phi^+\overline{v_h(\xi,\cdot)}, A^+_{\mu/h}\phi^+\overline{v_h(\xi,\cdot)}\big) \;=\; \left(\lim_{\delta,\varepsilon\to 0^+}\mathcal{R}_{\delta,\varepsilon}(\xi) + \lim_{\delta,\varepsilon,\beta\to 0^+}\mathcal{I}_{\delta,\varepsilon,\beta}(\xi)\right)\,, \tag{6.12}$$

where

$$\begin{aligned}
\mathcal{R}_{\delta,\varepsilon}(\xi) &:= \int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+} v(x)\overline{v(y)}\,(\phi(x)-\phi(y))^2\,\theta^{\delta,\varepsilon}_{\mu/h}(|x-y|)\,dx\,dy\,,\\
\mathcal{I}_{\delta,\varepsilon,\beta}(\xi) &:= \int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+}\phi(x)^2\big(2|v(x)|^2 - v(x)\overline{v(y)} - \overline{v(x)}v(y)\big)e_\beta(x)e_\beta(y)\,\theta^{\delta,\varepsilon}_{\mu/h}(|x-y|)\,dx\,dy\,.
\end{aligned}$$

As shown below, integrating $\lim_{\delta,\varepsilon\to 0^+}\mathcal{R}_{\delta,\varepsilon}(\xi)$ in (6.11) results in the remainder $R_{\mu,h}(\phi)$, satisfying the estimate stated in the lemma, whereas the second term in (6.12) combined with the second term in (6.11) yields the two leading terms in the expansion of $\operatorname{Tr}\rho\phi H^+_{\mu,h}\phi$.

We have

$$\mathcal{I}_{\delta,\varepsilon,\beta}(\xi) \;=\; \int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+}\Big[\frac12\Big(\mathcal{M}_\beta(\xi,x,y) + \overline{\mathcal{M}_\beta(\xi,x,y)}\Big) + \mathcal{N}_\beta(\xi,x,y)\Big]\theta^{\delta,\varepsilon}_{\mu/h}(|x-y|)\,dx\,dy\,,$$

where

$$\begin{aligned}
\mathcal{M}_\beta(\xi,x,y) \;&:=\; \Big(\phi(x)^2v(x)e_\beta(x) - \phi(y)^2v(y)e_\beta(y)\Big)\Big(\overline{v(x)}e_\beta(x) - \overline{v(y)}e_\beta(y)\Big)\,,\\
\mathcal{N}_\beta(\xi,x,y) \;&:=\; \Big(\phi(x)^2|v(x)|^2e_\beta(x) - \phi(y)^2|v(y)|^2e_\beta(y)\Big)\Big(e_\beta(y) - e_\beta(x)\Big)\,.
\end{aligned}$$

First, we show that

$$\lim_{\beta\to 0^+}\int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+}\mathcal{N}_\beta(\xi,x,y)\,\theta^{\delta,\varepsilon}_{\mu/h}(|x-y|)\,dx\,dy \;=\; 0\,. \tag{6.13}$$

Pointwise, we have $\lim_{\beta\to 0^+}\mathcal{N}_\beta(\xi,x,y) = 0$. In order to find a β-independent integrable upper bound, we separately consider the regions where $|x-y|$ is smaller and where $|x-y|$ is larger than some $r>0$. For $|x-y|>r$, we have

$$\big|\mathcal{N}_\beta(\xi,x,y)\,\theta^{\delta,\varepsilon}_{\mu/h}(|x-y|)\big| \;\leqslant\; Ch^{-d}|\xi'|\,\big\|F_{\mu/|\xi'|,\xi_d}\big\|^2_\infty\,\big(\phi(x)^2+\phi(y)^2\big)\,|\theta^{\delta,\varepsilon}_{\mu/h}(|x-y|)|\,, \tag{6.14}$$

uniformly in β. This is integrable in the region where $|x-y| > r$, because $\phi \in C_0^1(\mathbb{R}^d)$ and

$$\int_{|z|>r} \theta^{\delta}_{\mu/h}(|z|)\, dz \;\leqslant\; C\int_r^{\infty} t^{-2} dt \;<\infty\,,$$

where we used that $\theta(t) \leqslant C\, t^{-(d+1)} e^{-t/2}$ by Lemma 31 in Appendix D.2.

Next, if $|x-y| \leqslant r$, then the condition that $x \in \operatorname{supp}\phi$ or $y \in \operatorname{supp}\phi$ implies that both x and y belong to $B_{R+r}(0)$, where $R>0$ is such that $\operatorname{supp}\phi \subset B_R(0)$. Since

$$\big|\phi(x)^2|v(x)|^2 - \phi(y)^2|v(y)|^2\big| \;\leqslant\; Ch^{-1}|\xi'|\,\big\|\nabla\big(\phi^2 F^2_{\mu/|\xi'|,\xi_d}\big)\big\|_{\infty}\,|x-y|$$

and for $\beta_1, \beta_2 \leqslant 1$

$$|e_\beta(x) - e_\beta(y)| \;\leqslant\; \|\nabla e_\beta\|_\infty\,|x-y| \;\leqslant \sup_{x\in\mathbb{R}^d_+}\big(2\beta_1|x'|e^{-\beta_1|x'|^2} + \beta_2 e^{-\beta_2 x_d}\big)\,|x-y| \leqslant 3|x-y|\,,$$

it follows for $|x-y| \leqslant r$ that

$$\big|\mathcal{N}_\beta(\xi,x,y)\,\theta^{\delta,\varepsilon}_{\mu}(|x-y|)\big| \;\leqslant\; Ch^{-1}|\xi'|\,\chi_{B_{R+r}(0)}(y)\,|x-y|^2\,\theta^{\delta,\varepsilon}_{\mu/h}(|x-y|) \tag{6.15}$$

uniformly in $\beta_1, \beta_2 \leqslant 1$. The right side is integrable in the region where $|x-y| < r$, since

$$|B_{R+r}(0)|\int_{|z|\leqslant r} |z|^2\theta^{\delta}_{\mu/h}(|z|)\, dz \;\leqslant\; C\int_0^r dt \;=\; Cr \;<\; \infty\,.$$

Thus, due to (6.14) and (6.15), equation (6.13) follows from dominated convergence.

Let $g_h^{\delta,\varepsilon}(x) := \frac{h}{\varepsilon}\, e^{-\delta x/h}(1-e^{-\varepsilon x/h})$. By using (E.28) again, we may apply Lemma 22,

$$\begin{aligned}
h&\int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+} \mathcal{M}_\beta(\xi,x,y)\,\theta^{\delta,\varepsilon}_{\mu/h}(|x-y|)\,dx\,dy \;=\; \Big(\phi^2\overline{v_h(\xi,\cdot)}e_\beta, g_h^{\delta,\varepsilon}\big(hA^+_{\mu/h}\big)\overline{v_h(\xi,\cdot)}e_\beta\Big)\\
&= \int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+} \overline{v_h(\zeta,x)}v_h(\xi,x)\,\phi(x)^2\,e_\beta(x)\,g_h^{\delta,\varepsilon}(a_\mu(\zeta))\,v_h(\zeta,y)\,\overline{v_h(\xi,y)}\,e_\beta(y)\,dy\,dx\,d\zeta\\
&= \frac{|\xi'|h^{-2d}}{(2\pi)^{2(d-1)}}\int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+}\int_{\mathbb{R}_+} |\zeta'|\,e^{-ix'(\xi'-\zeta')/h}\,\phi(x)^2\,e_\beta(x)\,g_h^{\delta,\varepsilon}(a_\mu(\zeta))\\
&\quad\times \tilde F(\xi,\zeta,h^{-1}x_d,h^{-1}y_d)\,e^{-\beta_2 y_d}\int_{\mathbb{R}^{d-1}} e^{-iy'(\zeta'-\xi')/h}e^{-\beta_1|y'|^2}dy'\,dy_d\,dx\,d\zeta\,,
\end{aligned}$$

where for $\xi,\zeta \in \mathbb{R}^d_+$, and $s,t>0$

$$\tilde F(\xi,\zeta,s,t) \;:=\; \left(\frac{2}{\pi}\right)^2 F_{\mu/|\xi'|,\xi_d}(|\xi'|s)\,F_{\mu/|\zeta'|,\zeta_d}(|\zeta'|s)\,F_{\mu/|\xi'|,\xi_d}(|\xi'|t)\,F_{\mu/|\zeta'|,\zeta_d}(|\zeta'|t)\,.$$

Since $\xi' \mapsto (2\pi h)^{-(d-1)}(\mathcal{F}^{(d-1)}e^{-\beta_1|\cdot|^2})(\xi'/2\pi h)$ defines an approximate identity in $\mathbb{R}^{d-1}$ with respect to $\beta_1>0$ (see Appendix D.1), it follows that

$$\begin{aligned}
h&\lim_{\beta_1\to 0^+}\int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+} \mathcal{M}_\beta(\xi,x,y)\,\theta^{\delta,\varepsilon}_{\mu/h}(|x-y|)\,dx\,dy\\
&= \frac{|\xi'|^2h^{-d-1}}{(2\pi)^{(d-1)}}\left(\frac{2}{\pi}\right)^2\int_{\mathbb{R}^d_+}\phi(x)^2e^{-\beta_2 x_d}\int_{\mathbb{R}_+} F_{\mu/|\xi'|,\xi_d}(h^{-1}|\xi'|y_d)\,F_{\mu/|\xi'|,\xi_d}(h^{-1}|\xi'|x_d)\\
&\quad\times e^{-\beta_2 y_d}\int_{\mathbb{R}_+} F_{\mu/|\xi'|,\zeta_d}(h^{-1}|\xi'|y_d)\,g_h^{\delta,\varepsilon}(a_\mu(\xi',\zeta_d))\,F_{\mu/|\xi'|,\zeta_d}(h^{-1}|\xi'|x_d)\,d\zeta_d\,dy_d\,dx\,.
\end{aligned}$$

Hence, by integrating against $\big(a_\mu - 1\big)_-^0$ (see (6.11)) and changing variables in the y_d-integration, we find

$$\begin{aligned}
&h\int_{\mathbb{R}^d_+} \big(a_\mu(\xi)-1\big)_-^0 \lim_{\delta,\varepsilon,\beta\to 0^+} \int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+} \mathcal{M}_\beta(\xi,x,y)\, \theta^{\delta,\varepsilon}_{\mu/h}(|x-y|)\,dx\,dy\,d\xi \\
&= \frac{h^{-d}}{(2\pi)^{(d-1)}}\frac{2}{\pi} \lim_{\delta,\varepsilon,\beta_2\to 0^+} \int_{\mathbb{R}^{d-1}}\int_{\mathbb{R}^d_+}\int_{\mathbb{R}_+} \Big(\mathit{\Pi}^*_{\mu/|\xi'|}\,|\xi'|\big(a_\mu(\xi',\cdot)-1\big)_-^0\, F_{\mu/|\xi'|,(\,\cdot\,)}(h^{-1}|\xi'|x_d)\Big)(t) \\
&\qquad \times e^{-h|\xi'|^{-1}\beta_2 t}\Big(\mathit{\Pi}^*_{\mu/|\xi'|}\, g_h^{\delta,\varepsilon}(a_\mu(\xi',\cdot))\, F_{\mu/|\xi'|,(\,\cdot\,)}(h^{-1}|\xi'|x_d)\Big)(t)\,dt\,\phi(x)^2\, e^{-\beta_2 x_d}\,dx\,d\xi', \\
&= \frac{h^{-d}}{(2\pi)^{(d-1)}}\frac{2}{\pi} \lim_{\delta,\varepsilon\to 0^+} \int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+} |\xi'|\big(a_\mu(\xi)-1\big)_-^0\, g_h^{\delta,\varepsilon}(a_\mu(\xi))\, F_{\mu/|\xi'|,\xi_d}(h^{-1}|\xi'|x_d)^2\,\phi(x)^2\,dx\,d\xi \\
&= \int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+} |\xi'|\big(a_\mu(\xi)-1\big)_-^0\, a_\mu(\xi)\,|v_h(\xi,x)|^2\,\phi(x)^2\,dx\,d\xi\,,
\end{aligned}$$

where we are allowed to take limits after the integration in ξ and change the order of integration, since $\xi \mapsto |\xi'|(a_\mu(\xi)-1)_-^0$ belongs to $L^1(\mathbb{R}^d_+)$ whenever $d \geqslant 2$.

Considering (6.13), integrating the second term in (6.12), and combining the result with the second term in (6.11), gives

$$\begin{aligned}
&\int_{\mathbb{R}^d_+} \big(a_\mu(\xi)-1\big)_-^0 \Big[h \lim_{\delta,\varepsilon,\beta\to 0^+} \mathcal{I}_{\delta,\varepsilon,\beta}(\xi) - \int_{\mathbb{R}^d_+} |v_h(\xi,x)|^2\,\phi(x)^2\,dx\Big]\,d\xi \\
&= \int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+} |\xi'|\big(a_\mu(\xi)-1\big)_-\,|v_h(\xi,x)|^2\,d\xi\;\phi(x)^2\,dx \\
&\overset{(6.5)}{=} \Lambda^{(1)}_\mu\, h^{-d}\int_{\mathbb{R}^d_+} \phi(x)^2 dx - h^{-d}\int_{\mathbb{R}^d_+} \mathcal{K}_\mu(h^{-1}x_d)\,\phi(x)^2\,dx\,.
\end{aligned}$$

It remains to prove the bound on the remainder $R_{\mu,h}(\phi)$ given by

$$\begin{aligned}
R_{\mu,h}(\phi) &= h\int_{\mathbb{R}^d_+} \big(a_\mu(\xi)-1\big)_-^0 \lim_{\delta,\varepsilon\to 0^+} \mathcal{R}_{\delta,\varepsilon}(\xi)\,d\xi \\
&= h\int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+} \big(a_\mu(\xi)-1\big)_-^0 v_h(\xi,x)\overline{v_h(\xi,y)}\,(\phi(x)-\phi(y))^2\,\theta_{\mu/h}(|x-y|)\,dx\,dy\,d\xi\,,
\end{aligned}$$

where we have used that by Lemma 31 and Lemma 33 (see Appendix D.2),

$$\big|\theta^{\delta,\varepsilon}_\nu(t)\big| \leqslant \sup_{\delta\in[0,c]}\left|\frac{d}{d\delta}\big(\delta\theta^\delta_\nu(t)\big)\right| \leqslant C_\nu\, t^{-(d+1)}$$

and $\int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+} (\phi(x)-\phi(y))^2|x-y|^{-(d+1)}\,dx\,dy < \infty$.

For $0<\sigma<\frac{1}{2}$ and $f \in H^{2\sigma}(\mathbb{R}^{d-1})\cap L^1(\mathbb{R}^{d-1})$ we have

$$\frac{|\xi'|^{2\sigma}}{h^{2\sigma}}\int_{\mathbb{R}^{d-1}} e^{i\xi' x'/h} f(x')\,dx' = \big(\mathcal{F}\mathcal{F}^{-1}|2\pi\cdot|^{2\sigma}\mathcal{F}f\big)\left(\tfrac{-\xi'}{2\pi h}\right) = \int_{\mathbb{R}^{d-1}} e^{i\xi' x'/h}\,(-\Delta)^\sigma f\,(x')\,dx'\,,$$

and therefore, by the definition of $v_h(\xi,h)$,

$$\begin{aligned}
R_{\mu,h}(\phi) = h^{1+2\sigma}&\int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+} |\xi'|^{-2\sigma}\big(a_\mu(\xi)-1\big)_-^0\, v_h(\xi,x)\,\overline{v_h(\xi,y)} \\
&\times(-\Delta_{x'})^\sigma\Big(\big(\phi(x)-\phi(y)\big)^2\theta_{\mu/h}(|x-y|)\Big)\,dx\,dy\,d\xi\,.
\end{aligned}$$

Since $|v_h(\xi,x)| \leqslant Ch^{-d/2}|\xi'|^{1/2}$ and

$$\int_{\mathbb{R}^d_+} |\xi'|^{1-2\sigma}\big(a_\mu(\xi)-1\big)^0_-\,d\xi \;\leqslant\; \int_{|\xi'|^2\leqslant 1+2\mu}\int_{\xi_d^2\leqslant(1+2\mu)/|\xi'|^2} |\xi'|^{1-2\sigma}\,d\xi_d\,d\xi'$$
$$=\; |\mathbb{S}^{d-2}|(1+2\mu)^{1/2}\int_0^{(1+2\mu)^{1/2}} t^{d-2-2\sigma}dt \;=\; \frac{|\mathcal{S}^{d-2}|}{d-1-2\sigma}(1+2\mu)^{(d-2\sigma)/2},$$

it follows that

$$|R_{\mu,h}(\phi)| \;\leqslant\; C_\sigma\,\frac{(1+\mu)^{(d-2\sigma)/2}}{h^{d-1-2\sigma}}\int_{\mathbb{R}^d_+}\int_{\mathbb{R}^d_+}\Big|(-\Delta_{x'})^\sigma\Big(\big(\phi(x)-\phi(y)\big)^2\theta_{\mu/h}(|x-y|)\Big)\Big|\,dx\,dy\,.$$

As is shown in Appendix F.2, for any $\sigma\in(0,\frac12)$ there exists a constant $C_\sigma>0$ such that for all $\nu>0$

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\Big|(-\Delta_{x'})^\sigma\Big(\big(\phi(x)-\phi(y)\big)^2\theta_\nu(|x-y|)\Big)\Big|\,dx\,dy \;\leqslant\; C_\sigma\,, \tag{6.16}$$

and therefore (6.10) follows, which finishes the proof of Lemma 24. □

Proof of Proposition 21. First, by Lemma 28 and Lemma 23 we have

$$\begin{aligned}-\mathrm{Tr}\,\big(\phi H^+_{\mu,h}\phi\big)_- \;&\geqslant\; -\mathrm{Tr}\,\phi\big(H^+_{\mu,h}\big)_-\phi \\ &= -h^{-d}\,\Lambda^{(1)}_\mu\int_{\mathbb{R}^d_+}\phi(x)^2dx + h^{-d+1}\int_{\mathbb{R}^d_+}\phi(x)^2h^{-1}\mathcal{K}_\mu(h^{-1}x_d)\,dx\,.\end{aligned} \tag{6.17}$$

Moreover, by Lemma 24 and the Variational Principle

$$\begin{aligned}-\mathrm{Tr}\,\big(\phi H^+_{\mu,h}\phi\big)_- \;&\leqslant\; \mathrm{Tr}\,\rho\phi H^+_{\mu,h}\phi \\ &=\; -h^{-d}\Lambda^{(1)}_\mu\int_{\mathbb{R}^d_+}\phi(x)^2\,dx \;+\; h^{-d+1}\int_{\mathbb{R}^d_+}\phi(x)^2h^{-1}\mathcal{K}_\mu(h^{-1}x_d)\,dx \;-\; R_{\mu,h}(\phi)\,,\end{aligned} \tag{6.18}$$

with ρ as in Lemma 24, and by (6.10), for each $\sigma\in(0,\frac12)$ there exists $C_\sigma>0$ such that

$$|R_{\mu,h}(\phi)| \;\leqslant\; C_\sigma\,(1+\mu)^{(d-2\sigma)/2}\,h^{-d+1+2\sigma}\,.$$

Similarly as in [24, (3.8)], recalling that $\Lambda^{(2)}_\mu=\int_0^\infty\mathcal{K}_\mu(t)\,dt$, we have for any $\delta_1\in(0,1)$

$$\begin{aligned}&\left|\int_{\mathbb{R}^d_+}\phi(x)^2h^{-1}\mathcal{K}_\mu(h^{-1}x_d)\,dx - \Lambda^{(2)}_\mu\int_{\mathbb{R}^{d-1}}\phi(x',0)^2\,dx'\right| \\ &= \left|\int_0^\infty\mathcal{K}_\mu(t)\int_{\mathbb{R}^{d-1}}\int_0^{th}\partial_s\phi(x',s)^2\,ds\,dx'dt\right| \\ &\leqslant \int_0^\infty|\mathcal{K}_\mu(t)|\left(\int_0^{th}ds\right)^{\delta_1}\left(\int_0^\infty\left|\int_{\mathbb{R}^{d-1}}\partial_s\phi(x',s)^2\,dx'\right|^{(1-\delta_1)^{-1}}ds\right)^{1-\delta_1} \\ &\leqslant C_{\delta_1}h^{\delta_1}\int_0^\infty t^{\delta_1}|\mathcal{K}_\mu(t)|\,dt \;\leqslant\; C_{\delta_1}(1+\mu)^{(d-\delta_1)/2}h^{\delta_1}\,,\end{aligned}$$

where the last inequality is due to Lemma 20. Hence, it follows from (6.17) that

$$
\begin{aligned}
&\operatorname{Tr}\left(\phi H^{+}_{\mu,h}\phi\right)_{-} - h^{-d}\,\Lambda^{(1)}_{\mu}\int_{\mathbb{R}^d_+}\phi(x)^2dx + h^{-d+1}\Lambda^{(2)}_{\mu}\int_{\mathbb{R}^{d-1}}\phi(x',0)^2\,dx' \\
&\leqslant h^{-d+1}\left|\int_{\mathbb{R}^d_+}\phi(x)^2h^{-1}\mathcal{K}_\mu(h^{-1}x_d)\,dx - \Lambda^{(2)}_{\mu}\int_{\mathbb{R}^{d-1}}\phi(x',0)^2\,dx'\right| \\
&\leqslant C_{\delta_1}\,(1{+}\mu)^{(d-\delta_1)/2}\,h^{-d+1+\delta_1}\,,
\end{aligned}
\tag{6.19}
$$

and from (6.18) that

$$
\begin{aligned}
&\operatorname{Tr}\left(\phi H^{+}_{\mu,h}\phi\right)_{-} - h^{-d}\,\Lambda^{(1)}_{\mu}\int_{\mathbb{R}^d_+}\phi(x)^2dx + h^{-d+1}\Lambda^{(2)}_{\mu}\int_{\mathbb{R}^{d-1}}\phi(x',0)^2\,dx' \\
&\geqslant -C_\sigma\,(1{+}\mu)^{(d-2\sigma)/2}h^{-d+1+2\sigma} \\
&\quad - h^{-d+1}\left|\int_{\mathbb{R}^d_+}\phi(x)^2h^{-1}\mathcal{K}_\mu(h^{-1}x_d)\,dx - \Lambda^{(2)}_{\mu}\int_{\mathbb{R}^{d-1}}\phi(x',0)^2\,dx'\right| \\
&\geqslant\; -C_{\delta_2}\,(1{+}\mu)^{(d-\delta_2)/2}h^{-d+1+\delta_2} - C_{\delta_1}\,(1{+}\mu)^{(d-\delta_1)/2}\,h^{-d+1+\delta_1}\,,
\end{aligned}
\tag{6.20}
$$

where $\delta_2 := 2\sigma$. □

7. Analysis at the boundary

From the straightening of the boundary (Proposition 11) and the analysis on the half-space (Proposition 21), we obtain

Proposition 25. *There exist $c, C > 0$ and for all $\delta_1, \delta_2 > 0$ there exist $C_{\delta_1}, C_{\delta_1,\delta_2} > 0$ such that for all real-valued $\phi \in C^1_0(\mathbb{R}^d)$ satisfying $\|\nabla\phi\|_\infty \leqslant Cl^{-1}$ supported in a ball of radius $0 < l \leqslant c$ intersecting $\partial\Omega$,*

$$
\begin{aligned}
&- C_{\delta_1,\delta_2}\Bigg((1{+}\mu)^{(d-\delta_1)/2}\frac{l^{d-1-\delta_1}}{h^{d-1-\delta_1}} + (1{+}\mu)^{(d-\delta_2)/2}\frac{l^{d-1-\delta_2}}{h^{d-1-\delta_2}} \qquad (7.1)\\
&\qquad\qquad + (1{+}\mu)^{d/2}\,w(l)^2\,\frac{l^{d-1}}{h^{d-1}} + (1{+}\mu)^{d/2}\,w(l)\,\frac{l^d}{h^d}\Bigg) \\
&\leqslant \operatorname{Tr}\left(\phi H^{\Omega}_{\mu,h}\phi\right)_{-} - h^{-d}\,\Lambda^{(1)}_{\mu}\int_\Omega\phi(x)^2dx + h^{-d+1}\,\Lambda^{(2)}_{\mu}\int_{\partial\Omega}\phi(x)^2d\sigma(x) \\
&\leqslant C_{\delta_1}\left((1{+}\mu)^{(d-\delta_1)/2}\frac{l^{d-1-\delta_1}}{h^{d-1-\delta_1}} + (1{+}\mu)^{d/2}\,w(l)^2\,\frac{l^{d-1}}{h^{d-1}} + (1{+}\mu)^{d/2}\,w(l)\,\frac{l^d}{h^d}\right), \qquad (7.2)
\end{aligned}
$$

where w denotes the modulus of continuity of $\partial\Omega$, see (3.1).

Proof. From Proposition 11 and Proposition 21, by rescaling ϕ, it follows that

$$\begin{aligned}
&\operatorname{Tr}\left(\phi H^{\Omega}_{\mu,h}\phi\right)_- - h^{-d}\Lambda^{(1)}_\mu \int_\Omega \phi(x)^2dx + h^{-d+1}\Lambda^{(2)}_\mu \int_{\partial\Omega}\phi(x)^2 d\sigma(x)\\
&= \operatorname{Tr}\left(\phi H^{+}_{\mu,h}\phi\right)_- - h^{-d}\Lambda^{(1)}_\mu \int_{\mathbb{R}^d_+} \phi(x)^2dx + h^{-d+1}\Lambda^{(2)}_\mu \int_{\mathbb{R}^{d-1}}\phi(x',0)^2\, dx'\\
&\quad + \left(\operatorname{Tr}\left(\phi H^{\Omega}_{\mu,h}\phi\right)_- - \operatorname{Tr}\left(\phi H^{+}_{\mu,h}\phi\right)_-\right) + h^{-d+1}\Lambda^{(2)}_\mu\left(\int_{\partial\Omega}\phi(x)^2d\sigma(x) - \int_{\mathbb{R}^{d-1}}\phi(x',0)^2\,dx'\right)\\
&\leqslant C_{\delta_1}(1+\mu)^{(d-\delta_1)/2}(h/l)^{-d+1+\delta_1} + C(1+\mu)^{d/2}\,w(l)\,l^dh^{-d} + C|\Lambda^{(2)}_\mu|\,w(l)^2\,l^{d-1}h^{-d+1}.
\end{aligned}$$

Since, by Lemma 20, $|\Lambda^{(2)}_\mu| \leqslant C(1+\mu)^{d/2}$, we obtain the upper bound in (7.2). Here, we use that rescaling ϕ by $\phi_l := \phi(x/l)$ results in $\operatorname{Tr}(\phi_l H^{\Omega}_{\mu,h}\phi_l)_- = \operatorname{Tr}(\phi H^{\Omega}_{\mu,h/l}\phi)_-$, as can be seen by using the integral representation (0.10). The lower bound follows along the same lines. □

8. Proofs of Theorem 1 and Theorem 2

8.1. **Proof of Theorem 1.** Let $\Omega\subset\mathbb{R}^d$ be a bounded open domain with $\partial\Omega\in C^1$. First, if $h\geqslant c$ for some $c>0$, then, for any $\varepsilon>0$, we have

$$\begin{aligned}
&\left|\operatorname{Tr}\left(H^{\Omega}_{\mu,h}\right)_- - \Lambda^{(1)}_\mu\,|\Omega|\,h^{-d} + \Lambda^{(2)}_\mu\,|\partial\Omega|\,h^{-d+1}\right|\\
&\leqslant 2\,\Lambda^{(1)}_\mu|\Omega|\,h^{-d} + \left|\Lambda^{(2)}_\mu\right|\,|\partial\Omega|\,h^{-d+1} \leqslant C_\varepsilon\,(1+\mu)^{d/2}\,h^{-d+1+\varepsilon}\,.
\end{aligned}$$

Here, the first inequality follows from $H^{\Omega}_{\mu,h} = \chi_\Omega H_{\mu,h}\chi_\Omega$ and, by the same argument as in the proof of Lemma 9,

$$\operatorname{Tr}\left(\chi_\Omega H_{\mu,h}\chi_\Omega\right)_- \leqslant \Lambda^{(1)}_\mu\,h^{-d}\int_{\mathbb{R}^d}\chi_\Omega(x)^2\,dx = \Lambda^{(1)}_\mu\,|\Omega|\,h^{-d}\,.$$

In the second inequality we use that, by an explicit computation, $\Lambda^{(1)}_\mu \leqslant C\,(1+\mu)^{d/2}$, and that, by Lemma 20, $|\Lambda^{(2)}_\mu| \leqslant C\,(1+\mu)^{d/2}$. Hence, it remains to prove the claim for small h.

For $u\in\mathbb{R}^d$ let $\phi_u\in C^1_0(\mathbb{R}^d)$ be given by (1.3). By Lemma 4, we have

$$\begin{aligned}
&\operatorname{Tr}\left(H^{\Omega}_{\mu,h}\right)_- - \Lambda^{(1)}_\mu|\Omega|\,h^{-d} + \Lambda^{(2)}_\mu|\partial\Omega|\,h^{-d+1}\\
&= \int_{\mathbb{R}^d}\mathcal{L}_{\mu,h}(\phi_u)\,\frac{du}{l(u)^d} + \operatorname{Tr}\left(H^{\Omega}_{\mu,h}\right)_- - \int_{\mathbb{R}^d}\operatorname{Tr}\left(\phi_u H^{\Omega}_{\mu,h}\phi_u\right)_-\frac{du}{l(u)^d}\,,
\end{aligned}\tag{8.1}$$

where

$$\mathcal{L}_{\mu,h}(\phi_u) := \operatorname{Tr}\left(\phi_u H^{\Omega}_{\mu,h}\phi_u\right)_- - \Lambda^{(1)}_\mu h^{-d}\int_\Omega\phi_u(x)^2dx + \Lambda^{(2)}_\mu h^{-d+1}\int_{\partial\Omega}\phi_u(x)^2d\sigma(x)\,.$$

Note that if $u\in\mathbb{R}^d\backslash\Omega$ and $\operatorname{supp}(\phi_u)\cap\partial\Omega=\emptyset$, then $\mathcal{L}_{\mu,h}(\phi_u)=0$. Hence, it suffices to find bounds for $\mathcal{L}_{\mu,h}(\phi_u)$ when u belongs to the bulk, $u\in U_1 := \{u\in\Omega \mid B_{l(u)}(u)\cap\partial\Omega=\emptyset\}$, and when u is close to the boundary of Ω, $u\in U_2 := \{u\in\mathbb{R}^d \mid B_{l(u)}(u)\cap\partial\Omega\neq\emptyset\}$. If $u\in U_2$ then it follows from $\delta(u)\leqslant l(u)$ that $l(u)\leqslant 3^{-1/2}l_0$. Therefore, by choosing l_0 small enough, we are allowed to apply Proposition 25. By Proposition 8, in the bulk we have

$$0 \geqslant \int_{U_1}\mathcal{L}_{\mu,h}(\phi_u)\,\frac{du}{l(u)^d} \geqslant -C\,(1+\mu)^{(d-1)/2}h^{-d+2}\int_{U_1} l(u)^{-2}\,du\,,$$

whereas near the boundary, by Proposition 25,

$$
\begin{aligned}
&- C_{\delta_1,\delta_2}\,(1+\mu)^{d/2} \int_{U_2} \left(\frac{l(u)^{-1-\delta_1}}{h^{d-1-\delta_1}} + \frac{l(u)^{-1-\delta_2}}{h^{d-1-\delta_2}} + \frac{w(l(u))^2 l(u)^{-1}}{h^{d-1}} + \frac{w(l(u))}{h^d} \right) du \\
&\quad \leqslant \int_{U_2} \mathcal{L}_{\mu,h}(\phi_u)\, \frac{du}{l(u)^d} \qquad (8.2)\\
&\quad \leqslant C_{\delta_1}\,(1+\mu)^{d/2} \int_{U_2} \left(\frac{l(u)^{-1-\delta_1}}{h^{d-1-\delta_1}} + \frac{w(l(u))^2 l(u)^{-1}}{h^{d-1}} + \frac{w(l(u))}{h^d} \right) du\,.
\end{aligned}
$$

By (1.24), we have $\int_{U_1} l(u)^{-2}\,du \leqslant C\,l_0^{-1}$ (since $U_1 \subset \Omega^*$). Moreover, if $u \in U_2$ then $3^{-1} l_0 < l(u) \leqslant 3^{-1/2} l_0$. Hence, by the same argument as in (1.23), it follows for all $\beta \in \mathbb{R}$ that $\int_{U_2} l(u)^\beta\,du \leqslant C\,l_0^{\beta+1}$. Therefore, by (8.2), Proposition 5, and (8.1), for all $h \leqslant l_0/8$,

$$
\begin{aligned}
&- C_{\delta_1,\delta_2}\,(1+\mu)^{d/2}\,h^{-d+1}\Big(l_0^{-1} h\,\mathfrak{S}_d(l_0/h) + l_0^{-\delta_1} h^{\delta_1} + l_0^{-\delta_2} h^{\delta_2} + w(l_0)^2 + w(l_0)\,l_0\,h^{-1} \Big) \\
&\leqslant \operatorname{Tr}\big(H^{\Omega}_{\mu,h}\big)_- - \Lambda^{(1)}_\mu |\Omega|\,h^{-d} + \Lambda^{(2)}_\mu |\partial\Omega|\,h^{-d+1} \qquad (8.3)\\
&\leqslant C_{\delta_1}\,(1+\mu)^{d/2}\,h^{-d+1}\Big(l_0^{-1} h\,\mathfrak{S}_d(l_0/h) + l_0^{-\delta_1} h^{\delta_1} + w(l_0)^2 + w(l_0)\,l_0\,h^{-1} \Big)\,.
\end{aligned}
$$

In the case when $\partial\Omega \in C^{1,\gamma}$, i.e. if $w(t) = Ct^\gamma$, we choose l_0 proportional to $h^{(1+\delta_1)/(1+\delta_1+\gamma)}$ for $d > 2$, so that

$$
h^{d-1} \left| \operatorname{Tr}\big(H^{\Omega}_{\mu,h}\big)_- - \Lambda^{(1)}_\mu |\Omega|\,h^{-d} + \Lambda^{(2)}_\mu |\partial\Omega|\,h^{-d+1} \right| \leqslant C_{\delta_1}\,(1+\mu)^{d/2}\,h^{\delta_1\gamma/(\gamma+1+\delta_1)}
$$

for all $\delta_2 = \delta_1 \in (0,1)$. Since $\varepsilon := \delta_1\gamma/(\gamma+1+\delta_1)$ takes any value in $(0, \gamma/(\gamma+2))$ by choosing $\delta_1 \in (0,1)$ appropriately, the error estimate in Theorem 1 follows. In the case of $d = 2$, we choose l_0 proportional to $h^{2/(\gamma+2)}$ and obtain

$$
h^{d-1} \left| \operatorname{Tr}\big(H^{\Omega}_{\mu,h}\big)_- - \Lambda^{(1)}_\mu |\Omega|\,h^{-d} + \Lambda^{(2)}_\mu |\partial\Omega|\,h^{-d+1} \right| \leqslant C_{\delta_1}\,(1+\mu)^{d/2}\,h^{\varepsilon}
$$

for all $\varepsilon \in (0, \gamma/(\gamma+2))$, since $h^{\gamma/(\gamma+2)}|\ln(h)|^{1/2} \leqslant C\,h^\varepsilon$ for all $\varepsilon \in (0, \gamma/(\gamma+2))$.

In the general case of domains with C^1 boundaries, let $l_0 = \alpha^{-1}h$, where $\alpha > 0$ is such that $8h \leqslant l_0 < \frac{1}{2}$, i.e. $2h < \alpha \leqslant \frac{1}{8}$. Then, for all $\delta_1 = \delta_2 \in (0,1)$, there exists $C > 0$ such that

$$
\begin{aligned}
r_\mu(h) &:= h^{d-1}(1+\mu)^{-d/2} \left| \operatorname{Tr}\big(H^{\Omega}_{\mu,h}\big)_- - \Lambda^{(1)}_\mu |\Omega|\,h^{-d} + \Lambda^{(2)}_\mu |\partial\Omega|\,h^{-d+1} \right| \\
&\leqslant C \left(\alpha^{\delta_1} \mathfrak{S}(\alpha^{-1}) + w\left(\frac{h}{\alpha}\right)^2 + \frac{1}{\alpha}\, w\left(\frac{h}{\alpha}\right) \right),
\end{aligned}
$$

whenever $0 < h < \alpha/2$ and $\mu > 0$.

Let $\varepsilon > 0$ and choose $0 < \alpha \leqslant \frac{1}{8}$ such that $\alpha^{\delta_1}\mathfrak{S}(\alpha^{-1}) < \varepsilon/(2C)$. Then, because of $w(t) \to 0$ as $t \to 0^+$, there exists $\delta > 0$ such that $h/\alpha < \delta$ implies $w\big(\frac{h}{\alpha}\big)^2 + \frac{1}{\alpha} w\big(\frac{h}{\alpha}\big) < \varepsilon/(2C)$. In particular,

$$
r_\mu(h) < \varepsilon \qquad \forall h < \min\{\alpha/2, \alpha\delta\}\,,
$$

and therefore, $r_\mu(h) \in o(1)$, uniformly in $\mu > 0$, as $h \to 0$.

8.2. **Proof of Theorem 2.** After substituting $\mu = hm$ in Theorem 1, it immediately follows from the inequalities (0.14) and (0.15) that

$$\begin{aligned} |r_m(h)| &= \Big| \sum_{n\in\mathbb{N}} \big(h\lambda_n - 1\big)_- - \Lambda_0^{(1)} \, |\Omega| \, h^{-d} + \Big(\Lambda_0^{(2)} |\partial\Omega| - C_d \, |\Omega| \, m\Big) \, h^{-d+1} \Big| \\ &\leqslant |R_{mh}(h)| + |\Omega| h^{-d} \left|\Lambda_\mu^{(1)} - \Lambda_0^{(1)} - C_d \, mh\right| + |\partial\Omega| \, h^{-d+1} \left|\Lambda_\mu^{(2)} - \Lambda_0^{(2)}\right| \\ &\leqslant |R_{mh}(h)| + C_\varepsilon(\Omega) \Big(m^2 h^{-d+2} + m^\delta h^{-d+1+\delta} \Big) \end{aligned}$$

for any $\delta \in (0,1)$. Thus, by Theorem 1, in the case of $\partial\Omega \in C^{1,\gamma}$,

$$|r_m(h)| \leqslant C_\varepsilon(\Omega) \left(m^\varepsilon + m^2 + (1+mh)^{d/2} \right) h^{-d+1+\varepsilon} \,,$$

and if $\partial\Omega \in C^1$, then

$$\begin{aligned} &(m^\delta + m^2 + (1+m)^{d/2})^{-1} |r_m(h)| \\ &\leqslant \; (1+m)^{-d/2} |R_{mh}(h)| + C_\varepsilon(\Omega) \big(h^{-d+2} + h^{-d+1+\varepsilon} \big) \; \in o(h^{-d+1}) \,, \end{aligned}$$

uniformly in $m > 0$, as $h \to 0^+$.

Appendix A. Fractional Sobolev spaces

Let $\Omega \subset \mathbb{R}^d$ be open, let $s \in (0,1)$, and let $H^s(\Omega)$ denote the fractional Sobolev space $W^{s,2}(\Omega)$, i.e.

$$H^s(\Omega) \,=\, \Big\{ u \in L^2(\Omega) \,\Big|\, \int_{\mathbb{R}^d} |\xi|^{2s} |\hat{u}(\xi)|^2 \, d\xi < \infty \Big\} \,,$$

with the norm $\|u\|_{H^s(\Omega)} \,=\, \|(1+|\cdot|^2)^{s/2}\hat{u}\|_2$, with respect to which $H^s(\Omega)$ is a Banach space (see [14, Prop. 4.24]). Equivalently (see for example [14, Prop. 4.17 & Def. 4.23] or [15, (2.1)]), $u \in H^s(\Omega)$ if and only if $u \in L^2(\Omega)$ and

$$[u]_{s,\Omega} \,:=\, \bigg(\int_\Omega \int_\Omega \frac{|u(x)-u(y)|^2}{|x-y|^{d+2s}} \, dx \, dy \bigg)^{1/2} \,<\, \infty \,, \tag{A.1}$$

where $[u]_{s,\Omega}$ is called the *Gagliardo semi-norm* of $u \in H^s(\Omega)$, and moreover, $\|\cdot\|_{H^s(\Omega)}$ is equivalent to the norm on $H^s(\Omega)$ given by $u \mapsto \|u\|_2 + [u]_{s,\Omega}$. Note that, in contrast to the definition above, this characterization of $H^s(\Omega)$ can easily be extended to $W^{s,p}(\Omega)$ for arbitrary $p \in (1,\infty)$ (see [15, (2.1)]). Also, let

$$H_0^s(\Omega) := \overline{C_0^\infty(\Omega)}^{\|\cdot\|_{H^s(\Omega)}} \,, \tag{A.2}$$

equipped with $\|\cdot\|_{H^s(\Omega)}$. In particluar, $H_0^s(\mathbb{R}^d) = H^s(\mathbb{R}^d)$, since $C_0^\infty(\mathbb{R}^d)$ is dense in $H^s(\mathbb{R}^d)$ (see for instance [1, Theorem 7.38]).

If $W(\Gamma)$ denotes a class of functions defined on a subset $\Gamma \subset \mathbb{R}^d$, then an open set $\Omega \subset \mathbb{R}^d$ is called an *extension domain for* W, if there exists a bounded linear map $E : W(\Omega) \to W(\mathbb{R}^d)$, such that $(Eu)|_\Omega = u$. By [14, Prop. 4.43], any open Lipschitz domain $\Omega \subset \mathbb{R}^d$ is an extension domain for H^s. Clearly, *any* open subset $\Omega \subset \mathbb{R}^d$ is an extension domain for H_0^s, since any $f \in H_0^s(\Omega)$ can be extended by 0 to $\mathbb{R}^d$.

By [15, Theorem 6.5], $H^s(\mathbb{R}^d)$ is continuously embedded in $L^q(\mathbb{R}^d)$ for any $q \in [2, p^\star]$, where $p^\star = 2d/(d-2s) > 2$ denotes the so-called *fractional critical exponent* for $p = 2$. Thus, if $\Omega \subset \mathbb{R}^d$ is an extension domain for H^s (resp. for H_0^s), there exists $C > 0$ just depending on $d \geqslant 2$ and Ω, such that for any $u \in H^s(\Omega)$ (resp. $u \in H_0^s(\Omega)$) we have $\|u\|_{L^q(\Omega)} \leqslant C\,\|u\|_{H^s(\Omega)}$ for all $q \in [2, p^\star]$, i.e. $H^s(\Omega)$ (resp. $H_0^s(\Omega)$) is continuously embedded in $L^q(\Omega)$ for any $q \in [2, p^\star]$ [15, Theorem 6.7]. Moreover, by [15, Corollary 7.2], if Ω is also bounded, then any bounded subset $B \subset L^2(\Omega)$, satisfying $\sup_{u \in B}[u]_{s,\Omega} < \infty$, is relatively compact in $L^q(\Omega)$ for all $q \in [1, p^\star]$.

As a consequence, we obtain

Lemma 26 (Compact embedding)**.** *If $\Omega \subset \mathbb{R}^d$ is a bounded open Lipschitz domain, then the embedding $H^s(\Omega) \hookrightarrow L^2(\Omega)$ is compact. The same is true when H^s is replaced by H_0^s, in which case Ω may be any open subset of $\mathbb{R}^d$.*

Proof. Let B be the unit ball in $H^s(\Omega)$. Since $\|u\|_2 \leqslant \|u\|_{H^s(\Omega)}$ for all $u \in H^s(\Omega)$, B is also bounded in $L^2(\Omega)$. Moreover, by the equivalence of $\|\cdot\|_{H^s(\Omega)}$ and $\|\cdot\|_2 + [\,\cdot\,]_{s,\Omega}$, there exists $C > 0$ such that $[u]_{s,\Omega} \leqslant C\|u\|_{H^s(\Omega)} \leqslant C$ for all $u \in B$, in particular $\sup_{u \in B}[u]_{s,\Omega} < \infty$. Thus, since Ω is an extension domain for H^s (resp. for H_0^s), B is relatively compact in $L^2(\Omega)$, which means that the embedding $H^s(\Omega) \hookrightarrow L^2(\Omega)$ (resp. $H_0^s(\Omega) \hookrightarrow L^2(\Omega)$) is compact. □

Note that this implies that the operator $A_m^\Omega = (\sqrt{-\Delta+m^2} - m)_D$ with form domain $H_0^{1/2}(\Omega)$ has compact resolvent (see for instance [48, Prop. 10.6]).

Appendix B. Parallel surfaces of Lipschitz boundaries

For a subset $\Gamma \subset \mathbb{R}^d$ and $r > 0$, the set $\Gamma_r := \{x \in \mathbb{R}^d \,|\, \mathrm{dist}(x, \Gamma) < r\}$ is called a *tubular neighbourhood of* Γ. The boundary $\partial\Gamma_r$ of a tubular neighbourhood is called a *parallel set* (or *surface*) of Γ.

Lemma 27. *Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain and let $\Gamma := \partial\Omega$. There exist $\varepsilon > 0$ and $C > 0$ such that*

$$\mathcal{H}^{d-1}(\partial\Gamma_r) \leqslant C \qquad \forall r \leqslant \varepsilon ,$$

where $\mathcal{H}^{d-1}$ denotes the $(d-1)$-dimensional Hausdorff measure.

Proof. By [36, Prop. 5.8], for a compact set $\Gamma \subset \mathbb{R}^d$ there exists a constant $C > 0$, such that

$$\mathcal{H}^{d-1}(\partial\Gamma_r) \leqslant C\, r^{d-1} N(\Gamma, r) \qquad \forall r > 0,$$

where $N(\Gamma, r)$ denotes the minimal number of balls of radius r needed to cover Γ. Clearly, there exists $C > 0$ such that $N(\Gamma, r) \leqslant C\,|\Gamma_r|\, r^{-d}$ for all $r > 0$ (see for example [41, 5.6]), where $|\Gamma_r|$ denotes the Lebesgue measure of the tubular neighbourhood Γ_r. The latter is related to the Minkowski m-content of Γ, given by $\mathcal{M}^m(\Gamma) = \lim_{r\to 0^+} r^{m-d}|\Gamma_r|$ for $0 \leqslant m \leqslant d$, whenever the limit exists. Since $\Gamma = \partial\Omega$ is a Lipschitz boundary, it is in particular $(d-1)$-rectifiable (see e.g. [41, 15.3]). Hence, by [19, 3.2.39], we have $\mathcal{M}^{d-1}(\Gamma) = \mathcal{H}^{d-1}(\Gamma)$, in particular $\lim_{r\to 0^+} |\Gamma_r| r^{-1}$ exists. Therefore there exists $\varepsilon > 0$ and $C > 0$ such that $|\Gamma_r| \leqslant Cr$ for all $r \leqslant \varepsilon$, which proves the claim. □

Appendix C. Trace formulas

C.1. **Assigning a trace to unbounded operators.** If $\rho \geqslant 0$ is a trace class operator with range in the form domain $\mathcal{D}(q_A)$ of a given self-adjoint operator $A \geqslant 0$ on a separable Hilbert space $\mathcal{H}$, then it has a singular value decomposition $\rho = \sum_{j\in I} \mu_j (\psi_j, \cdot)\psi_j$, where $\{\psi_j\}_{j\in I} \subset \mathcal{D}(q_A)$ is an orthonormal set and $\mu_j \geqslant 0$ for all $j \in I$. Since $A^{1/2}\rho A^{1/2} \geqslant 0$, we may consider the (probably infinite) quantity

$$\sum_{k\in J} \left(\varphi_k, A^{1/2}\rho A^{1/2}\varphi_k\right), \tag{C.1}$$

where $\{\varphi_k\}_{k\in J}$ is an orthonormal basis in $\mathcal{H}$ with $\varphi_k \in \mathcal{D}(q_A) = \mathcal{D}(A^{1/2})$. Clearly, if A is bounded, then $\mathcal{D}(q_A) = \mathcal{H}$, and ρA is trace class, so that $\mathrm{Tr}\, A^{1/2}\rho A^{1/2} = \mathrm{Tr}\, \rho A$. Since

$$\sum_{k\in J} \left(\varphi_k, A^{1/2}\rho A^{1/2}\varphi_k\right) = \sum_{j\in I} \mu_j \sum_{k\in J} \left|\left(\varphi_k, A^{1/2}\psi_j\right)\right|^2 = \sum_{j\in I} \mu_j \|A^{1/2}\psi_j\|^2 ,$$

the quantity (C.1) does not depend on the choice of the orthonormal basis even if A is unbounded, and therefore we may write

$$\mathrm{Tr}\, \rho A := \mathrm{Tr}\, A^{1/2}\rho A^{1/2} = \sum_{k\in J} \left(\varphi_k, A^{1/2}\rho A^{1/2}\varphi_k\right) = \sum_{j\in I} \mu_j\, q_A(\psi_j) . \tag{C.2}$$

More generally, for a self-adjoint operator A with A_+ or A_- being bounded, at least one of the quantities $\mathrm{Tr}\, \rho A_+$ or $\mathrm{Tr}\, \rho A_-$ is finite. Hence, in this case, we define

$$\mathrm{Tr} \rho A := \mathrm{Tr} \rho A_+ - \mathrm{Tr} \rho A_- . \tag{C.3}$$

C.2. **Lieb Variational Principle for the sum of negative eigenvalues.** If H is a self-adjoint operator in a Hilbert space, such that $H \geqslant -c$ for some $c > 0$, and if the negative part of the spectrum of H consists entirely of eigenvalues, say $\{E_j\}_{j\in J}$, then [38]

$$-\operatorname{Tr}(H)_- \;=\; \sum_{j\in J} E_j \;=\; \inf_{0\leqslant\rho\leqslant\mathbb{I}} \operatorname{Tr}\rho H\,, \tag{C.4}$$

where the infimum is taken over all trace class operators ρ with $0 \leqslant \rho \leqslant 1$ and with range in the form domain of H. Indeed,

$$\inf_{0\leqslant\rho\leqslant\mathbb{I}} \operatorname{Tr}\rho H \;=\; \inf_{\{\psi_k\}_{k\in I}\ \mathrm{ONS},\, 0\leqslant\mu_k\leqslant 1} \sum_{k\in I} \mu_k\, q_H(\psi_k) \;\leqslant\; \sum_{j\in J} q_H(\varphi_j) \;=\; \sum_{j\in J} E_j\,,$$

where $\{\varphi_j\}_{j\in J}$ are the eigenfunctions corresponding to the eigenvalues $\{E_j\}_{j\in J}$. On the other hand, if $\sum_{k\in I}\mu_k(\psi_k,\cdot)\psi_k$ is the singular value decomposition of a trace class operator ρ with $0\leqslant\rho\leqslant\mathbb{I}$, then

$$\operatorname{Tr}\rho H \;=\; \sum\nolimits_{k\in I}\mu_k\, q_H(\psi_k) \geqslant -\sum\nolimits_{k\in I}\mu_k\, q_{(H)_-}(\psi_k) \;\geqslant\; -\sum\nolimits_{k\in I} q_{(H)_-}(\psi_k) \;\geqslant\; -\operatorname{Tr}\big(H\big)_-\,,$$

where $q_{(H)_-}$ denotes the quadratic form of the negative part of H.

Lemma 28. *If H is a self-adjoint operator in $L^2(D)$ for some $D\subset\mathbb{R}^d$ and satisfies the assumptions in Section C.2, then*

$$\operatorname{Tr}\left(\phi H\phi\right)_- \;\leqslant\; \operatorname{Tr}\phi(H)_-\phi \tag{C.5}$$

for all real-valued $\phi\in C_0^1(\mathbb{R}^d)$.

Proof. By the Variational Principle, we have

$$\begin{aligned}\operatorname{Tr}\left(\phi H\phi\right)_- \;&=\; -\inf_{0\leqslant\rho\leqslant\mathbb{I}}\operatorname{Tr}\rho\phi H\phi = \sup_{0\leqslant\rho\leqslant\mathbb{I}}\Big(\operatorname{Tr}\rho\phi(H)_-\phi - \operatorname{Tr}\rho\phi(H)_+\phi\Big)\\ &\leqslant\; \sup_{0\leqslant\rho\leqslant\mathbb{I}}\operatorname{Tr}\rho\phi(H)_-\phi \;\leqslant\; \operatorname{Tr}\phi(H)_-\phi\,,\end{aligned}$$

since $0\leqslant(\phi(H)_\pm\phi)^{1/2}\rho\,(\phi(H)_\pm\phi)^{1/2}\leqslant\phi(H)_\pm\phi$ for all ρ with $0\leqslant\rho\leqslant\mathbb{I}$ and range in the form domain of $\phi H\phi$. ☐

Appendix D. Special functions

D.1. **Approximate identities.** For completeness, we provide a short proof of the following well-known result, which is used several times in the main part of this thesis (proofs of Lemma 10 and Lemma 23). It describes the construction of sequences in $L^1(\mathbb{R}^d)$ converging to the Dirac measure on $\mathbb{R}^d$ in a weak sense.

Lemma 29. *For $\eta\in L^1(\mathbb{R}^d)$ real-valued with $\|\eta\|_1 = 1$, define the family $(\eta_\varepsilon)_{\varepsilon>0}\subset L^1(\mathbb{R}^d)$ by $\eta_\varepsilon(x) := \varepsilon^{-d}\,\eta(x/\varepsilon)$. Then $\|\eta_\varepsilon\|_1 = 1$ for all $\varepsilon>0$, and if $f\in L^\infty(\mathbb{R}^d)$ then $\int_{\mathbb{R}^d} f\eta_\varepsilon$ is uniformly bounded in ε. Moreover,*

$$\lim_{\varepsilon\to 0^+}\int_{\mathbb{R}^d}\eta_\varepsilon(x)f(x)\,dx \;=\; f(0)\,, \tag{D.1}$$

for any $f\in C(\mathbb{R}^d)\cap L^\infty(\mathbb{R}^d)$.

Proof. A simple change of variables yields $\int_{\mathbb{R}^d} f\,\eta_\varepsilon = \int_{\mathbb{R}^d} f(\varepsilon x)\eta(x)\,dx$. By choosing $f{=}1$, this already proves $\|\eta_\varepsilon\|_1 = \|\eta\|_1 = 1$. Also, whenever $f \in L^\infty(\mathbb{R}^d)$, then $|\int_{\mathbb{R}^d} f\eta_\varepsilon| \leqslant \|f\|_\infty$ uniformly in ε. The latter inequality also justifies the application of dominated convergence in order to prove (D.1) for $f \in C(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$. □

A family of functions $(\eta_\varepsilon)_{\varepsilon>0}$ is called an *approximate identity in* $\mathbb{R}^d$ *with respect to* η, if $(\eta_\varepsilon)_{\varepsilon>0}$ and η satisfy the assumptions of Lemma 29.

Example. A commonly used family of approximate identities are Gaussians, as they often appear as Fourier transforms of a Gaussian that has been introduced to regularize a given integral (see for instance (2.5) or (6.6)). Since for $\xi \in \mathbb{R}^d$ and $\alpha > 0$, we have

$$\big(\mathcal{F}e^{-\alpha|\cdot|^2}\big)(\xi) \;=\; \Big(\frac{\pi}{\alpha}\Big)^{d/2} e^{-\pi^2|\xi|^2/\alpha} \;=\; \frac{1}{(\sqrt{\alpha}/\pi)^d}\,\beta\big(\xi/(\sqrt{\alpha}/\pi)\big)\,, \tag{D.2}$$

where $\beta := \pi^{-d/2}e^{-|\cdot|^2}$, it follows that the Gaussians $\beta_\alpha^{(d)} := \mathcal{F}e^{-\alpha|\cdot|^2}$ form an approximate identity $(\beta_\alpha^{(d)})_{\alpha>0}$.

D.2. **Modified Bessel Functions of the Second Kind.** For $\beta \in \mathbb{R}$, solutions $s \mapsto K_\beta(s)$ to the Modified Bessel Equation $s^2y'' + sy' - (s^2 + \beta^2)\,y = 0$ are called Modified Bessel Functions of the Second Kind. For $s > 0$, as is shown for example in [52, (9.42)], we have

$$K_\beta(s) \;=\; \frac{s^\beta}{2^{\beta+1}} \int_0^\infty e^{-t-s^2/(4t)}\, t^{-\beta-1} dt\,, \tag{D.3}$$

and by changing variables, see [52, (9.43)], also

$$K_\beta(s) \;=\; \frac{\sqrt{\pi}}{\Gamma\big(\beta+\frac12\big)} \Big(\frac{s}{2}\Big)^\beta \int_1^\infty e^{-st}\,(t^2{-}1)^{\nu-1/2} dt\,. \tag{D.4}$$

In this thesis, we are interested in the values $\beta = (n{+}1)/2$ for $n \in \mathbb{N}$. In that case, these representations yield

Lemma 30. *For any* $n \in \mathbb{N}$, $\nu > 0$, *and* $s > 0$, *we have*

$$K_{(n+1)/2}(\nu s) \;=\; \Big(\frac{s}{\nu}\Big)^{(n+1)/2} \int_0^\infty e^{-\nu^2 t - s^2/(4t)}\,(2t)^{-(n+3)/2}\,dt \tag{D.5}$$

and for any $\alpha \in (0,2]$,

$$K_{(n+\alpha)/2}\big(\nu^{1/\alpha}s\big) = \Big(\frac{s}{\nu^{1/\alpha}}\Big)^{(n+\alpha)/2} \int_0^\infty e^{-\nu^{2/\alpha}t - s^2/(4t)}(2t)^{-(n+\alpha)/2-1}\,dt\,. \tag{D.6}$$

Moreover,

$$K_{(n+1)/2}(s) \;=\; \frac12 \Big(\frac{s}{2\pi}\Big)^{(n-1)/2} \int_{\mathbb{R}^n} e^{-s\sqrt{|p|^2+1}}\,dp\,. \tag{D.7}$$

Proof. The identities (D.5) and (D.6) follow directly from (D.3) by changing variables. For (D.7), we note that

$$\begin{aligned}\int_{\mathbb{R}^n} e^{-s\sqrt{|p|^2+1}}dp &= |\mathbb{S}^{n-1}| \int_0^\infty e^{-s\sqrt{r^2+1}}\, r^{n-1}\, dr \\ &= \frac{2\pi^{n/2}}{\Gamma(\frac{n}{2})} \int_1^\infty e^{-st}(t^2-1)^{(n-2)/2}\, t\, dt \\ &= \frac{\pi^{n/2}}{\Gamma(\frac{n}{2}+1)} \int_1^\infty e^{-st}\frac{d}{dt}(t^2-1)^{n/2}\, dt \\ &= \frac{\pi^{n/2}}{\Gamma(\frac{n}{2}+1)}\, s \int_1^\infty e^{-st}(t^2-1)^{n/2}\, dt \\ &= 2\left(\frac{2\pi}{s}\right)^{(n-1)/2} K_{(n+1)/2}(s)\,,\end{aligned}$$

where the last equality is due to (D.4). □

The following Lemma is used in the proof of Lemma 12.

Lemma 31. *For each $n \in \mathbb{N}_0$ there is a constant $C > 0$ such that for all $s > 0$*

$$K_{(n+1)/2}(s) \leqslant C\, s^{-(n+1)/2} e^{-s/2}\,. \tag{D.8}$$

Proof. If $n = 0$, then the estimate holds trivially, since $K_{1/2}(s) = \frac{\sqrt{\pi}}{2}\, s^{-1/2}e^{-s} < Cs^{-1/2}e^{-s/2}$. In the case $n \geqslant 1$, it follows from the integral representation (D.7) and the estimate

$$\begin{aligned}\int_{\mathbb{R}^n} e^{-s\sqrt{|p|^2+1}}dp &= |\mathbb{S}^{n-1}| \int_0^\infty e^{-s\sqrt{t^2+1}} t^{n-1} dt \\ &\leqslant |\mathbb{S}^{n-1}|\, e^{-s/2} \int_0^\infty e^{-st/2} t^{n-1} dt = C\, e^{-s/2}\, s^{-n}\,,\end{aligned}$$

that $K_{(n+1)/2}(s) \leqslant C\, s^{-(n+1)/2}e^{-s/2}$. □

Lemma 32. *For $d \in \mathbb{N}$ and $s \geqslant 0$, we have*

$$s\, K_{(d+3)/2}(s) \leqslant 2\, K_{(d+1)/2}\big(s/\sqrt{2}\big)\,. \tag{D.9}$$

Proof. We use the integral representation (D.7) with $n = d + 2$. For $p \in \mathbb{R}^{d+2}$, we write $p = (p_d, p_2)$, with $p_d \in \mathbb{R}^d$ and $p_2 \in \mathbb{R}^2$. Then, $(\sqrt{|p_d|^2+1} - |p_2|)^2 \geqslant 0$ implies that

$$\sqrt{|p|^2+1} \geqslant \tfrac{1}{\sqrt{2}}\left(\sqrt{|p_d|^2+1} + |p_2|\right).$$

Hence, by using (D.7) we obtain for $s > 0$,

$$\begin{aligned}K_{(d+3)/2}(s) &= \tfrac{s}{4\pi}\left(\tfrac{s}{2\pi}\right)^{(d-1)/2} \int_{\mathbb{R}^{d+2}} e^{-s\sqrt{|p|^2+1}}\, dp \\ &\leqslant \tfrac{s}{4\pi}\left(\tfrac{s}{2\pi}\right)^{(d-1)/2} \int_{\mathbb{R}^d} e^{-\frac{s}{\sqrt{2}}\sqrt{|p_d|^2+1}}\, dp_d \int_{\mathbb{R}^2} e^{-\frac{s}{\sqrt{2}}|p_2|}\, dp_2 \\ &= s\, K_{(d+1)/2}\big(s/\sqrt{2}\big) \int_0^\infty e^{-\frac{s}{\sqrt{2}}r}\, r\, dr = 2s^{-1} K_{(d+1)/2}\big(s/\sqrt{2}\big)\,.\end{aligned}$$

Since in the case $s = 0$ the inequality (D.9) is trivially true, this proves the claim. □

Lemma 33 (Derivative)**.** *For $\beta \in \mathbb{R}$ and $s > 0$, we have*

$$\frac{d}{ds} K_\beta(s) = \frac{\beta}{s} K_\beta(s) - K_{\beta+1}(s)\,. \tag{D.10}$$

Proof. This follows immediately from (D.3), since we are allowed to differentiate under the integral sign, due to

$$\left| \frac{\partial}{\partial s} \left(e^{-t-s^2/(4t)}\, t^{-\beta-1} \right) \right| = \frac{s}{2}\, e^{-t-s^2/(4t)}\, t^{-\beta-2} \leqslant \frac{b}{2}\, e^{-t-a^2/(4t)} t^{-\beta-2}$$

for all $t > 0$ and $s \in [a,b] \subset (0,\infty)$. $\square$

Appendix E. Lévy processes, Dirichlet forms, and Bernstein functions

This section gives a short overview of notions from the theory of stochastic processes and related topics in probability theory. We will not give all definitions in their full generality, but rather focus on the special cases we need in order to state and use the results in [37]. In particular, some of the stated results for Lévy processes also hold for a larger class of stochastic processes called Hunt processes, and in some cases even for all Markov processes. Our main references are [2], [33], and [47].

E.1. **Lévy processes and their transition operators.** Let $(\Gamma, \mathcal{F}, \mathbb{P})$ be a probability space, and let $\mathbb{R}^d$ be equipped with its Borel σ-algebra $\mathcal{B}(\mathbb{R}^d)$. We denote the probability distribution $\mathbb{P} \circ Y^{-1}$ of a random variable $Y : \Gamma \to \mathbb{R}^d$ by μ_Y.

A family $X = (X_t)_{t \geqslant 0}$ of random variables $X_t : \Gamma \to \mathbb{R}^d$ is called a *stochastic process* with time parameter set $[0,\infty)$ and state space $\mathbb{R}^d$. A stochastic process X is called a *Lévy process*, if (*i*) $X_0 = 0$ almost surely, (*ii*) X has independent[11] and stationary[12] increments, and (*iii*) it is stochastically continuous[13].

As is shown in [2, Proposition 1.4.4], if X is a Lévy process, then the probability distributions $\mu_t := \mu_{X_t}$ form a convolution semigroup $(\mu_t)_{t \geqslant 0}$, called the *convolution semigroup associated to X*.

By [33, 3.6.4], for any convolution semigroup $(\mu_t)_{t \geqslant 0}$ of finite measures on $\mathbb{R}^d$, there exists a unique function $\eta : \mathbb{R}^d \to \mathbb{C}$, such that

$$\int_{\mathbb{R}^d} e^{i\xi \cdot x}\, \mu_t(dx) \;=\; e^{-t\,\eta(\xi)} \tag{E.1}$$

for all $\xi \in \mathbb{R}^d$ and $t \geqslant 0$. Since a probability measure μ is uniquely determined by its Fourier transform $\xi \mapsto \int_{\mathbb{R}^d} e^{i\xi \cdot x} \mu(dx)$, also called the characteristic function of μ, it follows for a convolution semigroup $(\mu_t)_{t \geqslant 0}$ associated to a Lévy process X, that the function η in (E.1) is uniquely determined by X. In this case, η is called the *Lévy symbol*, *Lévy exponent*, or *characteristic exponent* of X.

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[11] A stochastic process X has *independent increments*, if for each $n \in \mathbb{N}$ and $0 \leqslant t_1 < \cdots < t_{n+1}$, the random variables $(X_{t_{k+1}} - X_{t_k})_{1 \leqslant k \leqslant n}$ are independent.

[12] The increments of a stochastic process X are called *stationary*, if for all $t > s \geqslant 0$, the random variable $X_t - X_s$ has the same probability distribution as $X_{t-s} - X_0$.

[13] A stochastic process X is called *stochastically continuous* in $t \geqslant 0$, if for any $\varepsilon > 0$ the probability of $|X_{t+h} - X_t|$ exceeding ε converges to 0 as $h \to 0$, i.e. $\lim_{h \to 0} \mathbb{P}(|X_{t+h} - X_t| > \varepsilon) = 0$. The process is called *stochastically continuous*, if it is stochastically continuous in the whole parameter space.

A common example is *(standard) Brownian motion*, also known as the *Wiener process*, which is a Lévy process $(B_t)_{t\geqslant 0}$ with continuous sample paths $t \mapsto B_t$, and such that $B_t - B_s$ is normally distributed with mean zero and variance $t-s$, whenever $0 \leqslant s \leqslant t$. It follows that

$$\mathbb{E}\big[e^{i\xi\cdot B_t}\big] \;=\; \int_{\mathbb{R}^d} e^{i\xi\cdot x} d\mu_{B_t}(x) \;=\; \frac{1}{(2\pi t)^{d/2}} \int_{\mathbb{R}^d} e^{i\xi\cdot x} e^{-|x|^2/(2t)}\,dx \;=\; e^{-t|\xi|^2/2}\,,$$

which means that $\eta(\xi) = |\xi|^2/2$ is the Lévy symbol of $(B_t)_{t\geqslant 0}$.

With each Lévy process X we may also associate a family of bounded operators $(T_t)_{t\geqslant 0}$, defined on the space $(B_b(\mathbb{R}^d), \|\cdot\|_\infty)$ of bounded Borel measurable functions on $\mathbb{R}^d$, by

$$T_t f(x) \;:=\; \int_{\mathbb{R}^d} f(x{+}y)\,\mu_t(dy) \;=\; \mathbb{E}[f(x{+}X_t)]\,. \tag{E.2}$$

They are known as the *transition operators* of the Lévy process X, since for any Borel set $E \subset \mathbb{R}^d$ and $x \in \mathbb{R}^d$, the quantity $p_t(x,E) := (T_t\chi_E)(x) = \mathbb{P}(x{+}X_t{\in}E)$ gives the probability of finding the process $x{+}X_t$ at time $t \geqslant 0$ in the set E after having started in x (since $X_0 = 0$). The *transition probability functions* p_t are *transition kernels*, which means that for any Borel set $E \subset \mathbb{R}^d$ the function $x \mapsto p_t(x,E)$ is Borel measurable, and for any $x \in \mathbb{R}^d$ the map $E \mapsto p_t(x,E)$ is a probability measure.

If the measures $p_t(x,\cdot)$ are absolutely continuous with respect to Lebesgue measure, i.e. if for all $t \geqslant 0$ and $x \in \mathbb{R}^d$ there exists a measurable function $y \mapsto \rho_t(x,y)$ such that $p_t(x,dy) = \rho_t(x,y)dy$, then X is said to have a *transition density* ρ_t. Since $p_t(x,E) = \mu_t(E{-}x)$, it follows that X has a transition density, if, for all $t \geqslant 0$, the probability distribution μ_t has a density f_t with respect to Lebesgue measure, and in this case $\rho_t(x,y) = f_t(y-x)$.

A Lévy process X is called *symmetric*, if $\mu_t(A) = \mu_t(-A)$ for all $t \geqslant 0$. Thus, if f_t is the density of a symmetric Lévy process with transition density ρ_t, then $f_t(x) = f_t(-x)$ and $\rho_t(x,y) = \rho_t(y,x)$.

By [2, 3.1.2], from Definition (E.2) and the properties of Lévy processes, it follows that $T_0 = I$, $T_{s+t} = T_sT_t$, $\|T_t\| \leqslant 1$ for all $s,t \geqslant 0$, as well as [2, 3.1.9]

$$\lim_{t\to 0+} \|T_t f - f\|_\infty \;=\; 0 \tag{E.3}$$

for all $f \in C_0(\mathbb{R}^d)$. Hence, $(T_t)_{t\geqslant 0}$ forms a one-parameter contraction semigroup of bounded operators in $B_b(\mathbb{R}^d)$, which is strongly continuous on the subspace $C_0(\mathbb{R}^d)$.

So far, we considered the transition operators T_t to be defined only on spaces of *bounded* functions. Moreover, many of the stated results are also true for a larger class of stochastic processes, called *Feller processes*. However, for Lévy processes, all the above properties can be carried over to $L^2(\mathbb{R}^d)$ (actually to $L^p(\mathbb{R}^d)$ for arbitrary $1 \leqslant p < \infty$, but we will only need the case $p{=}2$). Indeed, as is shown in [2, 3.4.2], if X is a Lévy process, then (E.2) defines a strongly continuous contraction semigroup[14] $(T_t)_{t\geqslant 0}$ of bounded linear maps in $L^2(\mathbb{R}^d)$. In particular, for all $f \in L^2(\mathbb{R}^d)$,

$$\lim_{t\to 0+} \|T_t f - f\|_2 \;=\; 0\,. \tag{E.4}$$

From now on, we call $(T_t)_{t\geqslant 0}$ the *contraction semigroup associated to* X, and unless specified otherwise, the operators T_t are defined on $L^2(\mathbb{R}^d)$.

[14] Since it will be clear from the context on which space the semigroup is defined, we use the same symbol for the transition operators on $B_b(\mathbb{R}^d)$ and on $L^2(\mathbb{R}^d)$.

E.2. **Generators, Dirichlet forms and killed Lévy processes.** The L^2-generator of the contraction semigroup $(T_t)_{t\geqslant 0}$ associated to a Lévy process X, i.e. the linear operator A defined on

$$\mathcal{D}(A) \;=\; \left\{\psi \in L^2(\mathbb{R}^d) : \exists \phi \in L^2(\mathbb{R}^d),\, \lim_{t\to 0+} \left\|\tfrac{1}{t}(T_t\psi - \psi) - \phi\right\|_2 = 0\right\}, \qquad \text{(E.5)}$$

by $A\psi := \lim_{t\to 0+} \frac{1}{t}(T_t\psi - \psi)$ for all $\psi \in \mathcal{D}(A)$, is also called the *generator of* X. As it is the case for the L^2-generator of any strongly continuous semigroup of bounded operators, $\mathcal{D}(A)$ is dense in $L^2(\mathbb{R}^d)$ [2, 3.2.6], and moreover, A is a closed operator [2, 3.2.7].

A Lévy process X is called *Lebesgue symmetric*, if its transition operators T_t are symmetric (hence self-adjoint) as operators in $L^2(\mathbb{R}^d)$. The generator A of a Lebesgue symmetric Lévy process is self-adjoint and negative semidefinite (see for instance [2, 3.4.6] or [47, A.13]), in particular $(-A)$ is positive semidefinite. Moreover, an approximation argument shows that a Lévy process is symmetric, if and only if it is Lebesgue symmetric (see [2, 3.4.10]).

The *Dirichlet (energy) form* of a symmetric Lévy process X is the closed quadratic form $\mathcal{E}$ on $L^2(\mathbb{R}^d)$ with domain $\mathcal{D}(\mathcal{E}) = \mathcal{D}((-A)^{1/2})$, defined by

$$\mathcal{E}(f) \;:=\; \left\|(-A)^{1/2} f\right\|_2^2\,, \qquad \text{(E.6)}$$

where A is the generator of X. There is an extensive theory around the concept of Dirichlet forms, also for more general classes of stochastic processes, see e.g. [25]. Dirichlet forms are also a good device for connecting with the theory of partial and pseudo-differential operators and their quadratic forms. Indeed, as we will see below, a large class of unbounded operators can be identified to be generators of symmetric Lévy processes, including the relativistic kinetic energy operator. Restrictions to domains of $\mathbb{R}^d$ with Dirichlet boundary condition is stochastically implemented by *killing* the underlying process.

For a Lévy process X and an open set $\Omega \subset \mathbb{R}^d$, define $\tau_\Omega := \inf\{t > 0 : X_t \notin \Omega\}$, which is known as the *first exit time* of X from Ω. Then, the *killed process* X^Ω, obtained by killing X when exiting Ω, is defined by

$$X_t^\Omega \;=\; \begin{cases} X_t\,, & t < \tau_\Omega \\ \partial\,, & t \geqslant \tau_\Omega \end{cases}\,, \qquad \text{(E.7)}$$

where ∂ is a so called *cemetry state*, which is some isolated point added[15] to the state space, in our case $\mathbb{R}^d$. It follows from the definition that X^Ω is again a Lévy process. If X is symmetric, then X^Ω is symmetric as well, and its Dirichlet form $(\mathcal{E}^\Omega, \mathcal{D}(\mathcal{E}^\Omega))$ is given by

$$\mathcal{D}(\mathcal{E}^\Omega) \;=\; \left\{u \in \mathcal{D}(\mathcal{E}) : u|_{\mathbb{R}^d\setminus\bar{\Omega}} \equiv 0\right\}, \qquad \text{(E.8)}$$

and $\mathcal{E}^\Omega(u) = \mathcal{E}(u)$ for all $u \in \mathcal{D}(\mathcal{E}^\Omega)$ (see [47, 12.49] and [25, p. 175]).

E.3. **Bernstein functions and related classes.** We say that a function $f \in C^\infty(\mathbb{R}_+, \mathbb{R})$ is a *Bernstein function*, if $f(s) \geqslant 0$ and $(-1)^{n-1} f^{(n)}(s) \geqslant 0$ for all $s > 0$ and $n \in \mathbb{N}$.

By [47, Theorem 3.2], a function $f : (0,\infty) \to \mathbb{R}$ is a Bernstein function, if and only if $\exists a, b \geqslant 0$ and a measure μ on $(0,\infty)$ satisfying[16] $\int_{(0,\infty)} (1 \wedge s)\, \mu(ds) < \infty$, such that f admits

[15] Any function on $\mathbb{R}^d$ is extended by zero to $\mathbb{R}^d \cup \{\partial\}$.

[16] Recall that $a \wedge b := \min\{a, b\}$ for $a, b \in \mathbb{R}$.

the *Lévy-Khintchine representation*

$$f(s) \;=\; a + bs + \int_{(0,\infty)} \big(1 - e^{-st}\big)\,\mu(dt)\,. \tag{E.9}$$

Then, (a, b, μ) is called the *characteristic triplet of* f, and the measure μ is called the Lévy measure of f. As an example, we may use the formula [2, 1.7]

$$t^\alpha = \frac{\alpha}{\Gamma(1-\alpha)} \int_0^\infty (1 - e^{-st})\, s^{-\alpha-1}\, ds \tag{E.10}$$

for $\alpha \in (0, 1)$ and $s \geqslant 0$, in order to see that $s \mapsto s^\alpha$ is a Bernstein function for all $\alpha \in [0, 1]$.

Closely related to Bernstein functions is the class of *completely monotone functions*, which is given by the set of all $g \in C^\infty(\mathbb{R}_+, \mathbb{R})$ satisfying $(-1)^n g^{(n)}(s) \geqslant 0$ for all $n \in \mathbb{N}_0$ and $s > 0$. Note that if f is a Bernstein function, then f' is completely monotone.

Completely monotone functions can be characterized by the Laplace transforms of measures on $[0, \infty)$ (see [47, Theorem 1.4]), more precisely for any completely monotone function g, there exists a unique measure μ on $[0, \infty)$, such that

$$g(s) \;=\; \int_{[0,\infty)} e^{-st}\,\mu(dt)\,. \tag{E.11}$$

A Bernstein function f is said to be *complete*, if its Lévy measure has a completely monotone density h with respect to the Lebesgue measure on $(0, \infty)$,

$$f(s) \;=\; a + bs + \int_{(0,\infty)} \big(1 - e^{-st}\big)\,h(t)\,dt\,. \tag{E.12}$$

On $\mathbb{R}^d$, the counterparts of completely monotone and Bernstein functions are given by the families of *positive definite functions* and *negative definite functions* (*in the sense of Bochner*), which we will denote by $C_P(\mathbb{R}^d)$ and $C_N(\mathbb{R}^d)$, respectively. In the literature, many authors use different equivalent definitions of these two classes (see for example [33, 3.5.3 and 3.6.5] or [47, 4.1 and 4.3]. For our purposes it suffices to use the following characterization of $C_P(\mathbb{R}^d)$, which is sometimes called *Bochner's theorem* [47, Theorem 4.11]: A continuous function ϕ on $\mathbb{R}^d$ is positive definite in the sense of Bochner, if and only if it is the characteristic function of a finite measure μ on $\mathbb{R}^d$, i.e. if $\phi(\xi) = \phi_\mu(\xi) = \int_{\mathbb{R}^d} e^{ix\cdot\xi}\mu(dx)$ for all $\xi \in \mathbb{R}^d$. Hence, the measure μ is uniquely determined by ϕ, and vice versa. Moreover (see [47, 4.4] or [33, 3.6.17]), a continuous function $\psi : \mathbb{R}^d \to \mathbb{C}$ is negative definite in the sense of Bochner, if and only if $\psi(0) \geqslant 0$ and $\xi \mapsto e^{-t\psi(\xi)}$ belongs to $C_P(\mathbb{R}^d)$ for all $t \geqslant 0$. For example, the function $\xi \mapsto |\xi|^2$ is negative definite, since the Gaussian $e^{-t|\xi|^2}$ is the characteristic function of a measure with a Gaussian density.

On $[0, \infty)$, the family of bounded continuous positive definite functions[17] coincides with the set of bounded completely monotone functions[18] [47, 4.9], and moreover, the family of continuous negative definite functions is the set of Bernstein functions [47, 4.10].

Continuous negative definite functions have a *Lévy-Khintchine representation* [47, 4.12]: A function η on $\mathbb{R}^d$ belongs to $C_N(\mathbb{R}^d)$, if and only if there exist $\alpha \geqslant 0$, $\beta \in \mathbb{R}^d$, a

[17]The notions of positive and negative definite functions can be defined on any abelian semigroup with involution, see [47, Ch. 4], in particular on $[0, \infty)$.

[18]Here, we use the convention that smooth functions on $(0, \infty)$ are continuously extended to $[0, \infty)$.

symmetric positive semi-definite matrix $Q \in \mathbb{R}^{d\times d}$, and a measure ν on $\mathbb{R}^d\setminus\{0\}$ satisfying $\int_{\mathbb{R}^d\setminus\{0\}}(1\wedge|y|^2)\,\nu(dy) < \infty$, such that

$$\eta(\xi) = \alpha + i\beta\cdot\xi + \xi\cdot Q\xi + \int_{\mathbb{R}^d\setminus\{0\}} \Big(1 - e^{i\xi\cdot y} + \frac{i\xi\cdot y}{1+|y|^2}\Big)\nu(dy)\,. \tag{E.13}$$

The quadruple (α,β,Q,ν) is uniquely determined by η, and vice versa.

E.4. **Characterization of Lévy processes and subordination.** The connection of the previous section to the theory of Lévy processes can be seen from (E.1). If η is the Lévy exponent of a Lévy process X, then for each $t \geqslant 0$, $\xi \mapsto e^{-t\eta(\xi)}$ is the characteristic function of the probability distribution $\mu_t = \mu_{X_t}$ of X_t, which is a finite measure on $\mathbb{R}^d$. Hence $e^{-t\eta}$ is positive definite, and it holds $\eta(0) = 0$, since $\mu_t(\mathbb{R}^d) = 1$ for all $t \geqslant 0$, which means that η is negative definite (see the characterization above). Moreover, as can be seen from the properties of $(\mu_t)_{t\geqslant 0}$ as a convolution semigroup of finite measures [33, 3.6.16], η is automatically continuous, and therefore $\eta \in C_N(\mathbb{R}^d)$.

As is shown in [34, 3.7.4], also the converse is true: Given $\eta \in C_N(\mathbb{R}^d)$ with $\eta(0) = 0$, there exists a unique Lévy process X, such that

$$\mathbb{E}\big[e^{i\xi\cdot X_t}\big] \;=\; e^{-t\eta(\xi)}\,. \tag{E.14}$$

Thus, there is a *one-to-one correspondence between Lévy processes and continuous negative definite functions vanishing at the origin*, given by (E.14). The characteristic quadrupel of a Lévy exponent η, given by the Lévy-Khintchine representation (E.13), takes the form $(0,\beta,Q,\nu)$. The triple (β,Q,ν) is therefore called the *characteristics* of the associated Lévy process X. For example, Brownian motion has characteristics $(0,I,0)$.

A Lévy process X with characteristics (b,Q,ν) is symmetric[19] (see [2, 3.4.11]) if and only if $b = 0$, ν is symmetric, i.e. $\nu(B) = \nu(-B)$ for all $B \in \mathcal{B}(\mathbb{R}^d\setminus\{0\})$, and its Lévy exponent is real-valued, i.e.

$$\eta(\xi) \;=\; \xi\cdot Q\xi + \int_{\mathbb{R}^d\setminus\{0\}} \Big(1 - \cos(\xi\cdot y)\Big)\nu(dy)\,. \tag{E.15}$$

The characterization of Lévy processes given by (E.14) immediately leads to the concept of subordination, considering the following fact from [33, 3.9.9]: If f is a Bernstein function and $\eta \in C_N(\mathbb{R}^d)$ takes values in $[0,\infty)$, then also $f\circ\eta \in C_N(\mathbb{R}^d)$.

If X is the Lévy process corresponding to η, and f is a Bernstein function with $f(0^+) = 0$, then the Lévy process X^f associated to $f\circ\eta$, is called the *Lévy process subordinate to X with respect to f*. Therefore, the subordinated Lévy process X^f satisfies

$$\mathbb{E}\big[e^{i\xi X_t^f}\big] \;=\; e^{-tf(\eta(\xi))}\,. \tag{E.16}$$

In the case of Lévy processes, this is a straightforward way of defining subordination. However, there is another approach, which can also be applied for larger classes of stochastic processes, and therefore is used in most of the literature on the subject. This alternative definition does not rely on the characterization given by (E.14), but makes use of so-called *subordinators* $(S_t)_{t\geqslant 0}$, one-dimensional Lévy processes that are non-decreasing (a.s.). Hence, if $(S_t)_{t\geqslant 0}$ is a subordinator, then $0 \leqslant S_{t_1} \leqslant S_{t_2}$ (a.s.), whenever $0 \leqslant t_1 \leqslant t_2$, which is why subordinators can be thought of as random models of time evolution. In fact, they are used to

[19] See Section E.2, in particular $-A$ is a positive semidefinite operator, where A is the generator of X.

change time in stochastic processes: If X is a Lévy process, then the process $X^S = (X_t^S)_{t\geqslant 0}$, defined by $X_t^S(\omega) := X_{S_t(\omega)}(\omega)$ for all $\omega \in \Gamma$, is also a Lévy process (see [2, 1.3.25]).

By [2, 1.3.15], there is one-to-one correspondence between subordinators and Bernstein functions f with $f(0+) = 0$, given by the Laplace transform: For a subordinator S, there exists a unique Bernstein function f, such that for all $u \geqslant 0$,

$$\mathbb{E}[e^{-uS_t}] \;=\; e^{-tf(u)} \,. \tag{E.17}$$

Conversely, if f is a Bernstein function with $f(0+) = 0$, then there exists a unique subordinator $(S_t)_{t\geqslant 0}$ satisfying (E.17). The Bernstein function corresponding to a subordinator S is called the *Laplace exponent of S*.

Now, if f is the Laplace exponent of a subordinator S, and η the Lévy symbol of a Lévy process X with $\eta(\xi) \geqslant 0$ for all $\xi \in \mathbb{R}^d$, then one can show (see [2, 1.3.27]), that $f \circ \eta$ is the Lévy symbol of X^S. This means that X^S coincides with the subordinated Lévy process X^f.

As an example, for any $\alpha \in [0, 2]$, consider the function $\xi \mapsto |\xi|^\alpha$, which is a continuous negative definite function on $\mathbb{R}^d$, since it is the convolution of the Bernstein function $s \mapsto s^{\alpha/2}$ and the continuous negative definite function $\xi \mapsto |\xi|^2$. The corresponding Lévy process is known as the *α-stable process* (see Section E.7 for the relativistic version).

E.5. **Fourier representation of Dirichlet energy forms.** For $\eta \in C_N(\mathbb{R}^d)$ and $s \geqslant 0$, we will use the following generalization of classical Sobolev spaces in $L^2(\mathbb{R}^d)$: The space $(H^{\eta,s}(\mathbb{R}^d), \|\cdot\|_{\eta,s})$, consisting of all $u \in L^2(\mathbb{R}^d)$ satisfying

$$\|u\|_{\eta,s} \;:=\; \big\|(1+|\eta(\cdot)|)^{s/2}\hat{u}\big\|_2 \;<\; \infty \,, \tag{E.18}$$

forms a Banach space (see [33, 3.10.3]). Note that, for $\eta(\xi) = |\xi|^\alpha$ with $\alpha \in [0, 2]$, the space $H^{\eta,s}(\mathbb{R}^d)$ coincides with the Sobolev space $H^{s\alpha/2}(\mathbb{R}^d)$ discussed in Appendix A.

Let η be the Lévy exponent of a symmetric Lévy process X. As is shown in [2, 3.3.3], the elements of the self-adjoint contraction semigroup $(T_t)_{t\geqslant 0}$ corresponding to X have the Fourier representation $T_t = \mathcal{F}^{-1} e^{-t\eta(2\pi\,\cdot)}\mathcal{F}$. This implies for the generator A of X, that $\mathcal{D}(A) = H^{\eta,2}(\mathbb{R}^d)$ and $-Au = \mathcal{F}^{-1}\eta(2\pi\,\cdot)\mathcal{F}u$ for all $u \in H^{\eta,2}(\mathbb{R}^d)$ (see [2, 3.4.4]). Thus, the Dirichlet energy form of X is given by

$$\mathcal{D}(\mathcal{E}) = H^{\eta,1}(\mathbb{R}^d) \,, \tag{E.19}$$

$$\mathcal{E}(u) \;=\; \int_{\mathbb{R}^d} \eta(2\pi\xi)\, |\hat{u}(\xi)|^2 \, d\xi \,. \tag{E.20}$$

This result allows the identification of many partial and pseudo-differential operators with generators of appropriate Lévy processes. In particular, many pseudo-differential operators which are functions of the Laplacian can be represented as generators of processes subordinate to Brownian motion. For example, the α-stable process from above is generated[20] by the fractional Laplacian $(-\Delta)^{\alpha/2}$, the positive semidefinite operator in $L^2(\mathbb{R}^d)$ defined by the quadratic form $u \mapsto \int_{\mathbb{R}^d} |2\pi\xi|^\alpha |\hat{u}(\xi)|^2 d\xi$ with form domain $H^{\alpha/2}(\mathbb{R}^d)$.

Since the Lévy exponent η of a symmetric Lévy process takes the form (E.15), the Fourier representation (E.20) of its Dirichlet energy form $\mathcal{E}$ implies that for all $u \in \mathcal{S}(\mathbb{R}^d)$,

$$\mathcal{E}(u) \;=\; \sum_{j,k=1}^d \tilde{Q}_{ij}\, \big(\partial_j u, \partial_k u\big)_2 + \int_{\mathbb{R}^d} \int_{\mathbb{R}^d\setminus\{0\}} \big|u(x+y) - u(x)\big|^2 \,\tilde{\nu}(dy)\, dx \,, \tag{E.21}$$

[20]For convenience, one uses the term *generator* for both A and the positive semidefinite operator $-A$.

for some symmetric positive semi-definite matrix $\tilde{Q} \in \mathbb{R}^{d\times d}$ and a measure $\tilde{\nu}$ on $\mathbb{R}^d\setminus\{0\}$, which differ only by constant factors from Q and ν in (E.15). The structure of (E.21) is not specific for Lévy processes, but a special case of the so-called *Beurling-Deny* formula (see [25, Theorem 3.2.1]). According to Beurling and Deny, a general Dirichlet form[21], satisfying a certain approximation property, can always be decomposed into a local[22] part and a non-local part. In (E.21), the first term is local, while the second term is non-local.

In the next section, we will state a similar result for Dirichlet energy forms of subordinated Lévy processes, together with explicit formulas for each of the parts in the decomposition. This allows to extract useful integral representations of the operators used in the main part of this work.

E.6. **Dirichlet energy forms of subordinated Lévy processes.** Let X be a symmetric Lévy process with transition probability functions p_t and corresponding contraction semi-group $(T_t)_{t\geqslant 0}$. Let f be a Bernstein function with characteristics $(0, 0, \mu)$, in particular $f(0+) = 0$, and let X^f denote the Lévy process subordinate to X with respect to f. By the Lévy-Khintchine formula (E.9),

$$f(s) \;=\; \int_{(0,\infty)} \left(1-e^{-st}\right) \mu(dt)\,. \tag{E.22}$$

As is shown in [44, Theorem 2.1], if $(\mathcal{E}^f, \mathcal{D}(\mathcal{E}^f))$ denotes the Dirichlet form of X^f, then (E.22) implies for all $u \in \mathcal{D}(\mathcal{E}^f)$ that $\mathcal{E}^f(u) = \int (u - T_t u, u)_2\, \mu(dt)$. This identity can be used to derive the following Beurling-Deny representation of $\mathcal{E}^f$ (see [44, Theorem 2.1 (2.11)]). For all $u \in \mathcal{D}(\mathcal{E}^f)$,

$$\mathcal{E}^f(u) \;=\; \int_{\mathbb{R}^d\times\mathbb{R}^d} |u(x) - u(y)|^2\, J^f(dx, dy), \tag{E.23}$$

where J^f is the positive measure Borel measure in $\mathbb{R}^d\times\mathbb{R}^d$ given by

$$J^f(B\times C) \;:=\; \frac{1}{2}\int_B \int_{(0,\infty)} p_s(x, C)\, \mu(ds)\, dx\,. \tag{E.24}$$

Let us add the remark, that (E.23) is a special case of a more general result discussed in [44], which also includes a term originating from the case $b \neq 0$ in the characteristic triplet $(0, b, \mu)$ of the Bernstein function f, which has the form $b\mathcal{E}(u)$. The validity of the formula, though, is then obviously restricted to $u \in \mathcal{D}(\mathcal{E}) \subset \mathcal{D}(\mathcal{E}^f)$.

E.7. **Example: Relativistic α-stable process.** We apply the above results in order to find an expression of the form (E.23) for the quadratic form

$$q_m^{\alpha,\Omega}(u) := \int_{\mathbb{R}^d} \left(\left(|2\pi\xi|^2 + m^{2/\alpha}\right)^{\alpha/2} - m\right) |\hat{u}(\xi)|^2\, d\xi$$

with form domain $\mathcal{D}(q_m^{\alpha,\Omega}) = H_0^{\alpha/2}(\Omega)$.

[21] As mentioned earlier, Dirichlet forms can be defined for a large class of stochastic processes, including processes with state spaces other than $\mathbb{R}^d$. See e.g. [25].

[22] A bilinear form B on $L^2(\mathbb{R}^d)$ is called *local*, if $B(u, v) = 0$ whenever $\operatorname{supp}(u) \cap \operatorname{supp}(v) = \emptyset$. Similarly, the corresponding quadratic form $u \mapsto B(u, u)$ is called local, if B is local.

Let X be the Lévy process corresponding to $\eta(\xi) = |\xi|^2$. This is the Lévy process generated by the Laplacian $(\Delta, H^2(\mathbb{R}^d))$, and, due to (E.6) and (E.19), the Dirichlet form of X is given by $(\mathcal{E}, H^1(\mathbb{R}^d))$, where $\mathcal{E}(u) = \|\nabla u\|_2^2$.

Since $\mathbb{E}[e^{i\xi\cdot X_t}] = e^{-t|\xi|^2}$, we have $X_t = B_{2t}$, where $(B_t)_{t\geqslant 0}$ denotes standard Brownian motion. Hence, X_t has the probability distribution $\mu_{X_t}(dx) = (4\pi t)^{-d/2} e^{-|x|^2/4t}\,dx$, and for any $t > 0$, the transition function p_t of X satisfies

$$p_t(x, E) \;=\; \mathbb{P}(x+X_t \in E) \;=\; (4\pi t)^{-d/2} \int_E e^{-|x-y|^2/4t}\,dy$$

for all $x \in \mathbb{R}^d$ and $E \in \mathcal{B}(\mathbb{R}^d)$. Therefore, $p_t(x, dy) = k_t(x, y)\,dy$, where k_t denotes the heat kernel in $\mathbb{R}^d$.

Next, for $m > 0$, let $f_\alpha : (0, \infty) \to \mathbb{R}$ be given by $f_\alpha(s) = (s+m^{2/\alpha})^{\alpha/2} - m$. By (E.10),

$$f_\alpha(s) \;=\; \frac{\alpha/2}{\Gamma(1-\alpha/2)} \int_0^\infty (1 - e^{-st})\, e^{-m^{2/\alpha}t}\, t^{-\alpha/2-1}\,dt\,. \tag{E.25}$$

Setting $\mu_\alpha(dt) := \frac{\alpha/2}{\Gamma(1-\alpha/2)} e^{-m^{2/\alpha}t} t^{-\alpha/2-1}\,dt$, which satisfies $\int_0^\infty (1\wedge t)\,\mu_\alpha(dt) < \infty$, we obtain that f_α is a Bernstein function with characteristic triplet $(0, 0, \mu_\alpha)$. We are interested in the Lévy process X^{f_α} subordinate to X with respect to f_α, which is known as the *relativistic α-stable process*.

By (E.19) and (E.20), the Dirichlet energy form of X^{f_α} is given by $(\mathcal{E}^{f_\alpha}, H^{f_\alpha(|\cdot|^2),1}(\mathbb{R}^d))$, where $H^{f_\alpha(|\cdot|^2),1}(\mathbb{R}^d) = H^{\alpha/2}(\mathbb{R}^d)$, and

$$\mathcal{E}^{f_\alpha}(u) \;=\; \int_{\mathbb{R}^d} \Big(\big(|2\pi\xi|^2 + m^{2/\alpha}\big)^{\alpha/2} - m \Big)\, |\hat{u}(\xi)|^2\,d\xi\,. \tag{E.26}$$

Now, let $X^{f_\alpha,\Omega}$ denote the Lévy process, obtained by killing X^{f_α} when leaving Ω, as was introduced in (E.7). The associated Dirichlet energy form, see (E.8), is given by

$$\mathcal{D}(\mathcal{E}^{f_\alpha,\Omega}) \;=\; \{u \in H^{\alpha/2}(\mathbb{R}^d) \,|\, u|_{\mathbb{R}^d\setminus\bar{\Omega}} \equiv 0\} \;=\; H_0^{\alpha/2}(\Omega),$$

and $\mathcal{E}^{f_\alpha,\Omega}(u) = \mathcal{E}^{f_\alpha}(u)$ for all $u \in \mathcal{D}(\mathcal{E}^{f_\alpha,\Omega})$. By (E.24),

$$\begin{aligned} J^{f_\alpha}(dx, dy) \;&=\; \frac{1}{2}\int_0^\infty k_t(x, y)\,\mu_\alpha(dt)\,dx\,dy \\ &=\; \frac{\alpha/2}{2\,\Gamma(1-\alpha/2)}\frac{1}{(4\pi)^{d/2}} \int_0^\infty e^{-m^{2/\alpha}t\,-\,|x-y|^2/4t}\, t^{-(d+\alpha)/2-1}\,dt\,dx\,dy \\ &\overset{(D.6)}{=}\; C_\alpha \Big(\frac{m^{1/\alpha}}{2\pi}\Big)^{(d+\alpha)/2} \frac{K_{(d+\alpha)/2}\big(m^{1/\alpha}|x-y|\big)}{|x-y|^{(d+\alpha)/2}}\,dx\,dy\,, \end{aligned}$$

where $C_\alpha := \frac{\alpha\, 2^{\alpha-1}\pi^{\alpha/2}}{\Gamma(1-\alpha/2)}$. Thus, due to (E.23), for all $u \in H_0^{\alpha/2}(\Omega)$, we have

$$q_m^{\alpha,\Omega}(u) \;:=\; C_\alpha \Big(\frac{m^{1/\alpha}}{2\pi}\Big)^{(d+\alpha)/2} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} |u(x)-u(y)|^2\, \frac{K_{(d+\alpha)/2}\big(m^{1/\alpha}|x-y|\big)}{|x-y|^{(d+\alpha)/2}}\,dx\,dy\,. \tag{E.27}$$

In particular, for $\alpha = 1$, we obtain (0.10), i.e.

$$\begin{aligned} q_m^\Omega(u) &= \Big(\frac{m}{2\pi}\Big)^{(d+1)/2} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} |u(x)-u(y)|^2\, \frac{K_{(d+1)/2}(m|x-y|)}{|x-y|^{(d+1)/2}}\,dx\,dy \\ &=: \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} |u(x)-u(y)|^2\, \theta_m(|x-y|)\,dx\,dy \end{aligned}$$

for all $u \in H_0^{1/2}(\Omega)$. This representation also follows from the corresponding integral representation of the kernel of $e^{-tA_m^\Omega}$, more precisely from (see [39, 7.11 – 7.12])

$$\frac{1}{t}\big((u,u)-(u,e^{-tA_m^\Omega}u)\big) \;=\; \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} |u(x)-u(y)|^2\,\theta_m\big((|x-y|^2+t^2)^{1/2}\big)\,dx\,dy. \tag{E.28}$$

Appendix F. Proofs of technical results

F.1. **Proof of (0.15).** In this section, we will prove that for each $\delta \in (0,1)$ there exists $C_\delta > 0$, such that

$$\big|\Lambda_\mu^{(2)} - \Lambda_0^{(2)}\big| \;\leqslant\; C_\delta\,\mu^\delta\,, \tag{0.15}$$

whenever $0 < \mu < \frac{1}{2}$.

For this, we will use details about $G_{\omega,\lambda}$, the second term in the expression (5.3) for $F_{\omega,\lambda}$, which have not been recorded in Lemma 16. More precisely, by [37, Theorem 1.1], for any $\omega \geqslant 0$, $G_{\omega,\lambda}$ is the Laplace transform of the measure

$$\gamma_{\omega,\lambda}(dr) \;=\; \chi_{(\sqrt{1+\omega^2},\infty)}(r)\,h_{\omega,\lambda}(r)\,dr\,, \tag{F.1}$$

where

$$h_{\omega,\lambda}(r) \;:=\; \frac{\lambda}{2\pi(\lambda^2+r^2)}\sqrt{\frac{r^2-1-\omega^2}{\lambda^2+1+\omega^2}}\;\exp\left[-\frac{1}{\pi}\int_0^\infty \frac{r}{r^2+s^2}\,\ln\left(\frac{1}{2}+\frac{1}{2}\sqrt{\frac{s^2+1+\omega^2}{\lambda^2+1+\omega^2}}\right)ds\right].$$

Note that

$$h_{\omega,\lambda}(r) \;=\; \frac{h_{0,\lambda/\sqrt{1+\omega^2}}\left(\frac{r}{\sqrt{1+\omega^2}}\right)}{\sqrt{1+\omega^2}}\,.$$

Lemma 34. *For all $r \geqslant 1$, the function $\lambda \mapsto h_{0,\lambda}(r)$ is differentiable, and*

$$\left|\frac{\partial}{\partial\lambda}h_{0,\lambda}(r)\right| \;\leqslant\; \frac{2}{\lambda}\,h_{0,\lambda}(r) \qquad \forall\lambda > 0\,. \tag{F.2}$$

Proof. We have

$$h_{0,\lambda}(r) \;=\; \frac{1}{2\pi}\frac{\lambda}{\lambda^2+r^2}\sqrt{\frac{r^2-1}{\lambda^2+1}}\;\exp\left[-\frac{1}{\pi}\int_0^\infty g_r(s,\lambda)\,ds\right] \;\geqslant 0\,,$$

where $g_r(s,\lambda) := \frac{r}{r^2+s^2}\,\ln\big(\frac{1}{2}+\frac{1}{2}\sqrt{\frac{s^2+1}{\lambda^2+1}}\big)$. Since

$$\frac{\partial g_r(s,\lambda)}{\partial\lambda} = -\frac{r}{r^2+s^2}\frac{\lambda}{\lambda^2+1}\frac{\sqrt{s^2+1}}{\sqrt{s^2+1}+\sqrt{\lambda^2+1}}\,,$$

and in particular $|\frac{\partial g_r(s,\lambda)}{\partial\lambda}| \leqslant \frac{r}{r^2+s^2}$, we are allowed to differentiate under the integral sign. Hence, by an explicit computation

$$\frac{\partial}{\partial\lambda}h_{0,\lambda}(r) \;=\; \left(1-\frac{2\lambda^2}{\lambda^2+r^2}-(1-I_{\lambda,r})\frac{\lambda^2}{\lambda^2+1}\right)\frac{h_{0,\lambda}(r)}{\lambda}\,,$$

where

$$I_{\lambda,r} \;:=\; \frac{1}{\pi}\int_0^\infty \frac{r}{r^2+s^2}\frac{\sqrt{s^2+1}}{\sqrt{s^2+1}+\sqrt{\lambda^2+1}}\,ds \;\leqslant\; \frac{1}{\pi}\int_0^\infty \frac{r}{r^2+s^2}\,ds \;=\; 1\,,$$

and thus, (F.2) follows. □

Proof of (0.15). As in the proof of Lemma 20, we study the t-integrals in regions for small and large t separately. For terms that are not absolutely integrable for large t, we integrate by parts in λ to produce factors of t^{-1}. We have

$$\begin{aligned}\Lambda_\mu^{(2)}-\Lambda_0^{(2)} &= \frac{2}{(2\pi)^d}\int_0^\infty\int_{\mathbb{R}^{d-1}}\int_0^\infty\Big[\big(|\xi'|\psi_{\mu/|\xi'|}(\lambda^2+1)-1\big)_-\Big(1-2F_{\mu/|\xi'|,\lambda}(t)^2\Big)\\ &\qquad -\big(|\xi'|\psi_0(\lambda^2+1)-1\big)_-\Big(1-2F_{0,\lambda}(t)^2\Big)\Big]\,d\lambda\,d\xi'\,dt\\ &= \frac{2}{(2\pi)^d}\int_0^\infty\int_{\mathbb{R}^{d-1}}\Big(\mathcal{I}^{(1)}_{\mu/|\xi'|}(|\xi'|,t)+\mathcal{I}^{(2)}_{\mu/|\xi'|}(|\xi'|,t)\Big)\,d\xi'\,dt\,, \end{aligned}\tag{F.3}$$

where, for $\omega,\nu>0$,

$$\begin{aligned}\mathcal{I}^{(1)}_\omega(\nu,t) &:= \int_0^\infty\Big(\big(\nu\,\psi_\omega(\lambda^2+1)-1\big)_- - \big(\nu\,\psi_0(\lambda^2+1)-1\big)_-\Big)\Big(1-2F_{\omega,\lambda}(t)^2\Big)\,d\lambda\,,\\ \mathcal{I}^{(2)}_\omega(\nu,t) &:= \int_0^\infty\big(\nu\,\psi_0(\lambda^2+1)-1\big)_-\Big(\big(1-2F_{\omega,\lambda}(t)^2\big)-\big(1-2F_{0,\lambda}(t)^2\big)\Big)\,d\lambda\,.\end{aligned}$$

We start with the integral of the second term, $\int_0^\infty\int_{\mathbb{R}^{d-1}}\mathcal{I}^{(2)}_{\mu/|\xi'|}(|\xi'|,t)\,d\xi'\,dt$. By using (5.27), i.e.

$$1-2F_{\omega,\lambda}(t)^2 = \cos\big(2\lambda t+2\vartheta_\omega(\lambda)\big)-4\sin\big(\lambda t+\vartheta_\omega(\lambda)\big)\,G_{\omega,\lambda}(t)-2G_{\omega,\lambda}(t)^2\,,$$

we obtain

$$\mathcal{I}^{(2)}_\omega(\nu,t) = \mathcal{I}^{(2a)}_\omega(\nu,t)-4\,\mathcal{I}^{(2b)}_\omega(\nu,t)-2\,\mathcal{I}^{(2c)}_\omega(\nu,t)\,,$$

where

$$\begin{aligned}\mathcal{I}^{(2a)}_\omega(\nu,t) &:= \int_0^\infty\big(\nu\,\psi_0(\lambda^2+1)-1\big)_-\Big(\cos\big(2\beta_{\omega,\lambda}(t)\big)-\cos\big(2\beta_{0,\lambda}(t)\big)\Big)\,d\lambda\,,\\ \mathcal{I}^{(2b)}_\omega(\nu,t) &:= \int_0^\infty\big(\nu\,\psi_0(\lambda^2+1)-1\big)_-\Big(\sin\big(\beta_{\omega,\lambda}(t)\big)\,G_{\omega,\lambda}(t)-\sin\big(\beta_{0,\lambda}(t)\big)\,G_{0,\lambda}(t)\Big)\,d\lambda\,,\\ \mathcal{I}^{(2c)}_\omega(\nu,t) &:= \int_0^\infty\big(\nu\,\psi_0(\lambda^2+1)-1\big)_-\int_0^\infty\Big(G_{\omega,\lambda}(t)^2-G_{0,\lambda}(t)^2\Big)d\lambda\,,\end{aligned}$$

and $\beta_{\omega,\lambda}(t):=\lambda t+\vartheta_\omega(\lambda)$. We have

$$\begin{aligned}\int_0^\infty|\mathcal{I}^{(2b)}_\omega(\nu,t)|\,dt &\leqslant \int_0^\infty\big(\nu\,\psi_0(\lambda^2+1)-1\big)_-\int_0^\infty\big|\sin\big(\beta_{\omega,\lambda}(t)\big)-\sin\big(\beta_{0,\lambda}(t)\big)\big|\,G_{\omega,\lambda}(t)\,dt\,d\lambda\\ &\quad+\int_0^\infty\big(\nu\,\psi_0(\lambda^2+1)-1\big)_-\int_0^\infty\big|\sin\big(\beta_{0,\lambda}(t)\big)\big|\big|G_{\omega,\lambda}(t)-G_{0,\lambda}(t)\big|\,dt\,d\lambda\,.\end{aligned}$$

Since by Lemma 18,

$$\begin{aligned}\left|\frac{\partial}{\partial\omega}\vartheta_\omega(\lambda)\right| &= \left|\frac{\partial}{\partial\omega}\,\vartheta_0\big(\tfrac{\lambda}{\sqrt{1+\omega^2}}\big)\right| = \left|\frac{\partial\vartheta_0}{\partial\lambda}\big(\tfrac{\lambda}{\sqrt{1+\omega^2}}\big)\right|\frac{\lambda\omega}{(1+\omega^2)^{3/2}}\\ &\leqslant \frac{\lambda}{\lambda^2+1+\omega^2}\frac{\omega}{\sqrt{1+\omega^2}} \leqslant \frac{1}{\sqrt{\lambda^2+1}} \leqslant 1\end{aligned}$$

for all $\lambda,\omega>0$, it follows that

$$\begin{aligned}\big|\sin\big(\beta_{\omega,\lambda}(t)\big)-\sin\big(\beta_{0,\lambda}(t)\big)\big| &\leqslant 2\left|\sin\Big(\tfrac{\beta_{\omega,\lambda}(t)-\beta_{0,\lambda}(t)}{2}\Big)\right|\\ &\leqslant 2\wedge\big|\vartheta_\omega(\lambda)-\vartheta_0(\lambda)\big| \leqslant 2\wedge\omega\,.\end{aligned}\tag{F.4}$$

Hence, by (5.39),

$$\int_0^\infty \big|\sin\big(\beta_{\omega,\lambda}(t)\big) - \sin\big(\beta_{0,\lambda}(t)\big)\big|\, G_{\omega,\lambda}(t)\, dt \;\leqslant\; 2(1\wedge\omega)\,(\lambda\wedge\lambda^{-1})\,. \tag{F.5}$$

Next, by (F.1), for any $\omega \geqslant 0$,

$$\begin{aligned}
\big|G_{\omega,\lambda}(t) - G_{0,\lambda}(t)\big| \;&=\; \left|\int_0^\infty e^{-tr}\left(\chi_{(\sqrt{1+\omega^2},\infty)}(r)\, h_{\omega,\lambda}(r) - \chi_{(1,\infty)}(r)\, h_{0,\lambda}(r)\right) dr\right| \\
&= \left|\int_0^\infty e^{-tr}\left(\chi_{(1,\infty)}\big(\tfrac{r}{\sqrt{1+\omega^2}}\big)\, \frac{h_{0,\lambda/\sqrt{1+\omega^2}}\big(\tfrac{r}{\sqrt{1+\omega^2}}\big)}{\sqrt{1+\omega^2}} - \chi_{(1,\infty)}(r)\, h_{0,\lambda}(r)\right) dr\right| \\
&= \left|\int_1^\infty \left(e^{-\sqrt{1+\omega^2}\,tr}\, h_{0,\lambda/\sqrt{1+\omega^2}}(r) - e^{-tr}\, h_{0,\lambda}(r)\right) dr\right| \\
&\leqslant \int_1^\infty e^{-tr}\left|h_{0,\lambda/\sqrt{1+\omega^2}}(r) - h_{0,\lambda}(r)\right| dr + \int_1^\infty \left|e^{-\sqrt{1+\omega^2}\,tr} - e^{-tr}\right|\, h_{0,\lambda}(r)\, dr\,.
\end{aligned}$$

By Lemma 34, for all $\omega \geqslant 0$,

$$\begin{aligned}
\left|\frac{\partial}{\partial\omega} h_{0,\lambda/\sqrt{1+\omega^2}}(r)\right| \;&=\; \left|\frac{\partial h_{0,\lambda}(r)}{\partial\lambda}\bigg|_{\frac{\lambda}{\sqrt{1+\omega^2}}}\; \frac{\lambda\omega}{(1+\omega^2)^{3/2}}\right| \\
&\leqslant\; \frac{2\omega}{1+\omega^2}\, h_{0,\lambda/\sqrt{1+\omega^2}}(r) \;\leqslant\; \frac{1}{\pi\sqrt{\lambda^2+1}}\, \frac{\lambda r}{\lambda^2+r^2}
\end{aligned}$$

and therefore,

$$\int_0^\infty\int_1^\infty e^{-tr}\left|h_{0,\lambda/\sqrt{1+\omega^2}}(r) - h_{0,\lambda}(r)\right| dr\, dt \;\leqslant\; \frac{\omega}{\pi\sqrt{\lambda^2+1}} \int_1^\infty \frac{\lambda}{\lambda^2+r^2}\, dr \;\leqslant\; \frac{\omega}{\sqrt{\lambda^2+1}}\,.$$

Since, again by (5.39),

$$\int_0^\infty\int_1^\infty \left|e^{-\sqrt{1+\omega^2}\,tr} - e^{-tr}\right|\, h_{0,\lambda}(r)\, dr\, dt \;\leqslant\; \omega \int_0^\infty G_{0,\lambda}(t)\, dt \;\leqslant\; \omega\,(\lambda\wedge\lambda^{-1})\,,$$

it follows that

$$\int_0^\infty \big|G_{\omega,\lambda}(t) - G_{0,\lambda}(t)\big|\, dt \;\leqslant\; 2\,(1\wedge\omega)\,(1\wedge\lambda^{-1})\,. \tag{F.6}$$

Since, for all $\omega \geqslant 0$, we have $1\wedge\omega \leqslant (1\wedge\omega)^\delta \leqslant \omega^\delta$ whenever $\delta \in (0,1)$, we obtain from (F.5) and (F.6)

$$\begin{aligned}
\int_0^\infty\!\!\int_{\mathbb{R}^{d-1}} \big|\mathcal{I}^{(2b)}_{\mu/|\xi'|}(|\xi'|,t)\big|\, d\xi'\, dt &\leqslant\; 4\,\mu^\delta \int_0^1 \nu^{d-2-\delta} \int_0^{\sqrt{\frac{1}{\nu^2}-1}} \big(1-\nu\,\psi_0(\lambda^2+1)\big)\;(1\wedge\lambda^{-1})\, d\lambda\, d\nu \\
&=\; 4\,\mu^\delta \int_0^1 \nu^{-\delta}\left(\int_0^1 d\lambda + \int_1^{1/\nu} \lambda^{-1}\, d\lambda\right) d\nu \\
&\leqslant\; 4\,\mu^\delta \int_0^1 \nu^{-\delta}\big(1+|\ln(\nu)|\big)\, d\nu \;=:\; C_\delta\,\mu^\delta
\end{aligned} \tag{F.7}$$

for all $\delta \in (0,1)$. Here, $0 < C_\delta < \infty$, since $\int_0^1 \nu^{-\delta}\, d\nu < \infty$ and $\int_0^1 \nu^{-\delta}|\ln(\nu)|\, d\nu < \infty$.

Similarly, since $G_{\omega,\lambda}(t) \leqslant \sin\vartheta_\omega(\lambda) \leqslant 1$, (F.6) also implies

$$\int_0^\infty\!\!\int_{\mathbb{R}^{d-1}} \big|\mathcal{I}^{(2c)}_{\mu/|\xi'|}(|\xi'|,t)\big|\, d\xi'\, dt \;\leqslant\; C_\delta\,\mu^\delta \tag{F.8}$$

for any $\delta \in (0,1)$.

Next, for $\mathcal{I}^{(2a)}_{\omega}(\nu,t)$, we write

$$\begin{aligned}&\int_0^\infty\!\!\int_{\mathbb{R}^{d-1}} \big|\mathcal{I}^{(2a)}_{\mu/|\xi'|}(|\xi'|,t)\big|\,d\xi'\,dt \\ &= \int_0^\infty \nu^{d-2}\bigg(\int_0^\nu \big|\mathcal{I}^{(2a)}_{\mu/\nu}(\nu,t)\big|\,dt + \int_\nu^1 \big|\mathcal{I}^{(2a)}_{\mu/\nu}(\nu,t)\big|\,dt + \int_1^\infty \big|\mathcal{I}^{(2a)}_{\mu/\nu}(\nu,t)\big|\,dt\bigg)\,d\nu\,.\end{aligned} \tag{F.9}$$

By (F.4), for any $\omega>0$, we have

$$\big|\cos\big(2\beta_{\omega,\lambda}(t)\big)-\cos\big(2\beta_{0,\lambda}(t)\big)\big| \;\leqslant\; 2\,\big|\sin\big(\beta_{\omega,\lambda}(t)-\beta_{0,\lambda}(t)\big)\big| \;\leqslant\; 2\wedge\omega\,, \tag{F.10}$$

and thus, for any $\delta\in(0,1)$,

$$\begin{aligned}&\int_0^\infty \nu^{d-2}\int_0^\nu\!\!\int_0^\infty\big(\nu\,\psi_0(\lambda^2+1)-1\big)_-\Big|\cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)-\cos\big(2\beta_{0,\lambda}(t)\big)\Big|\,d\lambda\,dt\,d\nu \\ &\leqslant 2\int_0^1\nu^{d-2}\int_0^\nu\int_0^{1/\nu}\big(1-\nu\,\psi_0(\lambda^2+1)\big)(1\wedge\mu/\nu)\,d\lambda\,dt\,d\nu \;\leqslant\; \mu^\delta\int_0^1\nu^{-\delta}\,d\nu \;=\; C_\delta\,\mu^\delta\,.\end{aligned}$$

In the region $t\in[\nu,1)$, we use (5.29), i.e.

$$\cos\big(2\beta_{\mu/\nu,t}(\lambda)\big) \;=\; \frac{1}{2t}\left(\frac{d}{d\lambda}\sin\big(2\beta_{\mu/\nu,t}(\lambda)\big)-2\cos\big(2\beta_{\mu/\nu,t}(\lambda)\big)\frac{d\vartheta_{\mu/\nu}}{d\lambda}\right)\,.$$

After integrating by parts, we obtain

$$\begin{aligned}&\int_0^1\nu^{d-2}\int_\nu^1\bigg|\int_0^{\sqrt{\frac{1}{\nu^2}-1}}\big(1-\nu\,\psi_0(\lambda^2+1)\big)\Big(\cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)-\cos\big(2\beta_{0,\lambda}(t)\big)\Big)\,d\lambda\bigg|dt\,d\nu \\ &\leqslant \int_0^1\nu^{d-1}\int_\nu^1\frac{1}{2t}\int_0^{\sqrt{\frac{1}{\nu^2}-1}}\frac{\lambda}{\sqrt{\lambda^2+1}}\Big|\sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)-\sin\big(2\beta_{0,\lambda}(t)\big)\Big|\,d\lambda\,dt\,d\nu \\ &\quad-\int_0^1\nu^{d-2}\int_\nu^1\frac{1}{t}\int_0^{\sqrt{\frac{1}{\nu^2}-1}}\Big|\cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)-\cos\big(2\beta_{0,\lambda}(t)\big)\frac{d\vartheta_0}{d\lambda}(\lambda)\Big|\,d\lambda\,dt\,d\nu\,.\end{aligned}$$

By (F.4), for any $\delta\in(0,1)$,

$$\begin{aligned}&\int_0^1\nu^{d-1}\int_\nu^1\frac{1}{2t}\int_0^{\sqrt{\frac{1}{\nu^2}-1}}\frac{\lambda}{\sqrt{\lambda^2+1}}\Big|\sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)-\sin\big(2\beta_{0,\lambda}(t)\big)\Big|\,d\lambda\,dt\,d\nu \\ &\leqslant \int_0^1\nu^{d-1}\int_\nu^1\frac{1}{2t}\int_0^{1/\nu}(1\wedge\mu/\nu)\,d\lambda\,dt\,d\nu \;\leqslant\; \mu^\delta\int_0^1\nu^{d-2-\delta}|\ln(\nu)|\,d\nu \;\leqslant\; C_\delta\,\mu^\delta\,.\end{aligned}$$

Moreover, since $\vartheta_\omega(\lambda)=\vartheta_0(\lambda/\sqrt{1+\omega^2})$, for any $\omega>0$, by Lemma 18 (properties of ϑ_ω),

$$\begin{aligned}\left|\frac{\partial}{\partial\omega}\left(\frac{d\vartheta_\omega}{d\lambda}(\lambda)\right)\right| \;&=\; \frac{\omega}{1+\omega^2}\left|\lambda\frac{d^2\vartheta_\omega}{d\lambda^2}(\lambda)+\frac{d\vartheta_\omega}{d\lambda}(\lambda)\right| \\ &\leqslant\; \frac{\omega}{1+\omega^2}\left(\frac{\lambda\sqrt{1+\omega^2}}{(\lambda^2+1+\omega^2)^{3/2}}+\frac{\sqrt{1+\omega^2}}{\lambda^2+1+\omega^2}\right) \;\leqslant\; \frac{2}{\lambda^2+1}\,,\end{aligned} \tag{F.11}$$

and therefore, by (F.10),

$$\begin{aligned}
&\int_0^1 \nu^{d-2}\int_\nu^1 \frac{1}{t}\int_0^{\sqrt{\frac{1}{\nu^2}-1}} \Big|\cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)-\cos\big(2\beta_{0,\lambda}(t)\big)\frac{d\vartheta_0}{d\lambda}(\lambda)\Big|\,d\lambda\,dt\,d\nu\\
&\leqslant \int_0^1 \nu^{d-2}\int_\nu^1 \frac{1}{t}\int_0^{1/\nu}\Big|\cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)-\cos\big(2\beta_{0,\lambda}(t)\big)\Big|\,\frac{d\vartheta_0}{d\lambda}(\lambda)\,d\lambda\,dt\,d\nu\\
&\quad+\int_0^1 \nu^{d-2}\int_\nu^1 \frac{1}{t}\int_0^{1/\nu}\Big|\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)-\frac{d\vartheta_0}{d\lambda}(\lambda)\Big|\,d\lambda\,dt\,d\nu\\
&\leqslant 3\int_0^1 \nu^{d-2}\int_\nu^1 \frac{1}{t}\int_0^{1/\nu}\frac{(1\wedge\mu/\nu)}{\lambda^2+1}\,d\lambda\,dt\,d\nu\\
&\leqslant 3\mu^\delta\int_0^1 \nu^{d-2-\delta}\int_\nu^1\frac{1}{t}\left(\int_0^1 d\lambda+\int_1^{1/\nu}\lambda^{-2}d\lambda\right)dt\,d\nu\\
&\leqslant 3\mu^\delta\int_0^1 \nu^{d-2-\delta}|\ln(\nu)|\,(2-\nu)\,d\nu\ \leqslant 3\mu^\delta\int_0^1\nu^{-\delta}|\ln(\nu)|\,d\nu\ \leqslant\ C_\delta\,\mu^\delta
\end{aligned}$$

for any $\delta\in(0,1)$. In the region where $t\in[1,\infty)$, by integrating by parts twice, we obtain

$$\begin{aligned}
&\int_0^1 \nu^{d-2}\int_1^\infty \left|\int_0^{\sqrt{\frac{1}{\nu^2}-1}}\big(1-\nu\,\psi_0(\lambda^2+1)\big)\Big(\cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)-\cos\big(2\beta_{0,\lambda}(t)\big)\Big)\,d\lambda\right|dt\,d\nu\\
&=\int_0^1 \nu^{d-1}\int_1^\infty \frac{1}{2t}\left|\int_0^{\sqrt{\frac{1}{\nu^2}-1}}\frac{\lambda}{\lambda^2+1}\left(\sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)-\sin\big(2\beta_{0,\lambda}(t)\big)\right)\,d\lambda\right|dt\,d\nu\\
&\quad+\int_0^1\nu^{d-2}\int_1^\infty\frac{1}{t}\left|\int_0^{\sqrt{\frac{1}{\nu^2}-1}}\Big(1-\nu\,\psi_0(\lambda^2+1)\Big)\right.\\
&\qquad\qquad\left.\times\left(\cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)-\cos\big(2\beta_{0,\lambda}(t)\big)\frac{d\vartheta_0}{d\lambda}(\lambda)\right)\,d\lambda\right|dt\,d\nu\\
&\leqslant\ \sum_{k=1}^5\int_0^1\nu^{d-2}\int_1^\infty\frac{1}{t^2}\,\big|J^{(k)}_{\mu/\nu}(\nu,t)-J^{(k)}_0(\nu,t)\big|\,dt\,d\nu\,,
\end{aligned}$$

where, for $\omega\geqslant 0$ and $0\leqslant\nu\leqslant 1$,

$$\begin{aligned}
J^{(1)}_\omega(\nu,t)\ &:=\ \frac{\nu^2}{4}\sqrt{\tfrac{1}{\nu^2}-1}\,\cos\big(2\beta_{\omega,(\nu^{-2}-1)^{1/2}}(t)\big)\,,\\
J^{(2)}_\omega(\nu,t)\ &:=\ \frac{\nu}{4}\int_0^{\sqrt{\frac{1}{\nu^2}-1}}\frac{1}{(\lambda^2+1)^{3/2}}\,\cos\big(2\beta_{\omega,\lambda}(t)\big)\,d\lambda\,,\\
J^{(3)}_\omega(\nu,t)\ &:=\ \nu\int_0^{\sqrt{\frac{1}{\nu^2}-1}}\frac{\lambda}{\sqrt{\lambda^2+1}}\,\frac{d\vartheta_\omega}{d\lambda}(\lambda)\,\sin\big(2\beta_{\omega,\lambda}(t)\big)\,d\lambda\,,\\
J^{(4)}_\omega(\nu,t)\ &:=\ \frac{1}{2}\int_0^{\sqrt{\frac{1}{\nu^2}-1}}\big(1-\nu\,\psi_0(\lambda^2+1)\big)\,\frac{d^2\vartheta_\omega}{d\lambda^2}(\lambda)\,\sin\big(2\beta_{\omega,\lambda}(t)\big)\,d\lambda\,,\\
J^{(5)}_\omega(\nu,t)\ &:=\ \int_0^{\sqrt{\frac{1}{\nu^2}-1}}\big(1-\nu\,\psi_0(\lambda^2+1)\big)\,\left(\frac{d\vartheta_\omega}{d\lambda}(\lambda)\right)^2\cos\big(2\beta_{\omega,\lambda}(t)\big)\,d\lambda\,.
\end{aligned}$$

By (F.10), we have

$$\big|J^{(1)}_\omega(\nu,t)-J^{(1)}_0(\nu,t)\big|\ \leqslant\ (1\wedge\omega)\,\frac{\nu}{2}$$

and

$$\left|J_\omega^{(2)}(\nu,t)-J_0^{(2)}(\nu,t)\right| \leqslant \frac{\nu}{2}\,(1\wedge\omega)\int_0^{1/\nu}\frac{1}{\lambda^2+1}\,d\lambda \leqslant \frac{\nu}{2}\,(1\wedge\omega)\,(2-\nu) \leqslant (1\wedge\omega)\,\nu\,.$$

By (F.11), similarly as above,

$$\left|J_\omega^{(3)}(\nu,t)-J_0^{(3)}(\nu,t)\right| \leqslant \nu\int_0^{1/\nu}\frac{1\wedge\omega}{\lambda^2+1}\,d\lambda \leqslant 2\,(1\wedge\omega)\,\nu\,.$$

For $J_\omega^{(4)}$, we compute

$$\begin{aligned}\frac{d^3\vartheta_0}{d\lambda^3} = {}& \frac{5\lambda^2+1}{\pi\lambda^2(\lambda^2+1)^3}\left(\frac{3\lambda^2+1}{\lambda}\,\tilde{l}_0(\lambda)-\sqrt{\lambda^2+1}\right)\\ &-\frac{1}{\pi\lambda(\lambda^2+1)^2}\left((3-\lambda^{-2})\,\tilde{l}_0(\lambda)+\frac{3\lambda^2+1}{\lambda\sqrt{\lambda^2+1}}-\frac{\lambda}{\sqrt{\lambda^2+1}}\right),\end{aligned}$$

where $\tilde{l}_0(\lambda)$ denotes the logarithm defined in (5.14), satisfying $\frac{\lambda}{\sqrt{\lambda^2+1}} \leqslant \tilde{l}_0(\lambda) \leqslant 1$. Thus

$$\begin{aligned}\left|\frac{d^3\vartheta_0}{d\lambda^3}\right| &\leqslant \frac{15}{\pi}\,\frac{1}{(\lambda^2+1)^2}+\frac{1}{\pi\lambda(\lambda^2+1)^2}\left(3\lambda+\frac{2\lambda}{\sqrt{\lambda^2+1}}+\frac{1}{\lambda\sqrt{\lambda^2+1}}-\frac{\tilde{l}_0(\lambda)}{\lambda^2}\right)\\ &\leqslant \frac{15}{\pi}\,\frac{1}{(\lambda^2+1)^2}+\frac{1}{\pi(\lambda^2+1)^2}\left(3+\frac{2}{\sqrt{\lambda^2+1}}\right) \leqslant \frac{20}{\pi}\,\frac{1}{(\lambda^2+1)^2}\end{aligned}$$

and therefore

$$\left|\frac{d^3\vartheta_\omega}{d\lambda^3}(\lambda)\right| = \frac{1}{(1+\omega^2)^{3/2}}\left|\frac{d^3\vartheta_0}{d\lambda^3}\Big(\tfrac{\lambda}{\sqrt{1+\omega^2}}\Big)\right| \leqslant \frac{20}{\pi}\,\frac{\sqrt{1+\omega^2}}{(\lambda^2+1+\omega^2)^2}\,.$$

Hence,

$$\begin{aligned}\left|\frac{\partial}{\partial\omega}\frac{d^2\vartheta_\omega}{d\lambda^2}(\lambda)\right| &= \left|\frac{\lambda\,\omega}{1+\omega^2}\,\frac{d^3\vartheta_\omega}{d\lambda^3}(\lambda)+\frac{2\,\omega}{1+\omega^2}\,\frac{d^2\vartheta_\omega}{d\lambda^2}(\lambda)\right|\\ &\leqslant \frac{26}{\pi}\,\frac{\omega}{1+\omega^2}\,\frac{\sqrt{1+\omega^2}}{(\lambda^2+1+\omega^2)^{3/2}} \leqslant \frac{26}{\pi}\,\frac{1}{(\lambda^2+1)^{3/2}}\,,\end{aligned}$$

since $\left|\frac{d^2\vartheta_\omega}{d\lambda^2}(\lambda)\right| \leqslant \frac{\sqrt{1+\omega^2}}{(\lambda^2+1+\omega^2)^{3/2}}$, and thus

$$\left|\frac{d^2\vartheta_\omega}{d\lambda^2}(\lambda)-\frac{d^2\vartheta_0}{d\lambda^2}(\lambda)\right| \leqslant C\,\frac{1}{\lambda^2+1}\,(1\wedge\omega)\,. \tag{F.12}$$

From (F.5) and (F.12), it follows that

$$\left|J_\omega^{(4)}(\nu,t)-J_0^{(4)}(\nu,t)\right| \leqslant C\int_0^{1/\nu}\frac{1\wedge\omega}{\lambda^2+1}\,d\lambda \leqslant C\,(1\wedge\omega)\,(2-\nu) \leqslant C\,(1\wedge\omega)\,.$$

Similarly, by (F.10), (F.11), and $0 \leqslant \frac{d\vartheta_\omega}{d\lambda}(\lambda) \leqslant \frac{1}{\sqrt{\lambda^2+1}}$,

$$\begin{aligned}\left|J_\omega^{(5)}(\nu,t)-J_0^{(5)}(\nu,t)\right| &\leqslant \int_0^{1/\nu}\frac{2}{\sqrt{\lambda^2+1}}\left|\frac{d\vartheta_\omega}{d\lambda}(\lambda)-\frac{d\vartheta_0}{d\lambda}(\lambda)\right|d\lambda\\ &\quad+\int_0^{1/\nu}\frac{1}{\lambda^2+1}\left|\cos\big(2\beta_{\omega,\lambda}(t)\big)-\cos\big(2\beta_{0,\lambda}(t)\big)\right|d\lambda\\ &\leqslant 6\int_0^{1/\nu}\frac{1\wedge\omega}{\lambda^2+1}\,d\lambda \leqslant 6\,(1\wedge\omega)\,.\end{aligned}$$

Combining the above estimates, we obtain, for any $\delta \in (0,1)$,

$$\sum_{k=1}^{5} \int_0^1 \nu^{d-2} \int_1^\infty \frac{1}{t^2} \left| J^{(k)}_{\mu/\nu}(\nu,t) - J^{(k)}_0(\nu,t) \right| dt\, d\nu \;\leqslant\; C\,\mu^\delta \int_0^1 \nu^{d-2-\delta} d\nu \;\leqslant\; C_\delta\, \mu^\delta\,, \tag{F.13}$$

and therefore, by (F.9),

$$\int_0^\infty \int_{\mathbb{R}^{d-1}} \left| \mathcal{I}^{(2a)}_{\mu/|\xi'|}(|\xi'|,t) \right| d\xi'\, dt \;\leqslant\; C_\delta\, \mu^\delta \tag{F.14}$$

for any $\delta \in (0,1)$.

For $\mathcal{I}^{(1)}_\omega(\nu,t)$, note that $\Gamma_0 \subset \Gamma_\mu$ for all $\mu > 0$, where

$$\Gamma_\mu := \left\{ (\nu,\lambda) \in \mathbb{R}_+ \times \mathbb{R}_+ \,|\, \nu^2(\lambda^2+1) \leqslant 1+2\mu \right\},$$

and therefore

$$\begin{aligned}
&\int_0^\infty \int_{\mathbb{R}^{d-1}} \mathcal{I}^{(1)}_{\mu/|\xi'|}(|\xi'|,t)\, d\xi'\, dt \\
&= \int_0^\infty \int_0^1 \nu^{d-1} \int_0^{\sqrt{\frac{1}{\nu^2}-1}} \big(\psi_0(\lambda^2+1) - \psi_{\mu/\nu}(\lambda^2+1)\big)\big(1-2F_{\mu/\nu,\lambda}(t)^2\big)\, d\lambda\, d\nu\, dt \\
&\quad + \int_0^\infty \int_1^{\sqrt{1+2\mu}} \nu^{d-2} \int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big)\big(1-2F_{\mu/\nu,\lambda}(t)^2\big)\, d\lambda\, d\nu\, dt \\
&\quad + \int_0^\infty \int_0^1 \nu^{d-2} \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big)\big(1-2F_{\mu/\nu,\lambda}(t)^2\big)\, d\lambda\, d\nu\, dt\,.
\end{aligned} \tag{F.15}$$

We use the same strategy as above, i.e. we consider the respective integrals in (F.15) of the three terms in (5.27) separately. While the terms containing a factor of $G_{\mu/\nu,\lambda}(t)$ can be controlled by using (5.39), i.e. $\int_0^\infty G_{\omega,\lambda}(t)\, dt \leqslant \lambda \wedge \lambda^{-1}$ for all $\omega \geqslant 0$, we use integration by parts in λ to deal with the terms only containing $\cos(2\beta_{\omega,\lambda}(t))$.

Since

$$\left| \frac{\partial}{\partial\omega} \psi_\omega(\lambda^2+1) \right| \;=\; 1 - \frac{\omega}{\sqrt{\lambda^2+1+\omega^2}} \;\leqslant\; 1\,,$$

we have $|\psi_\omega(\lambda^2+1) - \psi_0(\lambda^2+1)| \;\leqslant\; \omega$, and therefore

$$\begin{aligned}
&\int_0^1 \nu^{d-1} \int_0^{\sqrt{\frac{1}{\nu^2}-1}} \int_0^\infty \left| \psi_0(\lambda^2+1) - \psi_{\mu/\nu}(\lambda^2+1) \right| G_{\mu/\nu,\lambda}(t)\, dt\, d\lambda\, d\nu \\
&\leqslant \mu \int_0^1 \nu^{d-2} \int_0^{1/\nu} (\lambda \wedge \lambda^{-1})\, d\lambda\, d\nu \;\leqslant\; \mu \int_0^1 \nu^{d-2} |\ln \nu|\, d\nu \;=\; C\,\mu\,.
\end{aligned}$$

Similarly,

$$\begin{aligned}
&\int_1^{\sqrt{1+2\mu}} \nu^{d-2} \int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \int_0^\infty \big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big)\, G_{\mu/\nu,\lambda}(t)\, dt\, d\lambda\, d\nu \\
&\leqslant \int_1^{\sqrt{1+2\mu}} \nu^{d-2} \int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \big(\lambda \wedge \lambda^{-1}\big)\, d\lambda\, d\nu \\
&\leqslant \frac{1}{2} \int_1^{\sqrt{1+2\mu}} \nu^{d-2} \left(\frac{1+2\mu}{\nu^2} - 1 \right) d\nu \;\leqslant\; \mu \int_1^{\sqrt{1+2\mu}} \nu^{d-4}\, d\nu \;\leqslant\; C\,\mu\,.
\end{aligned}$$

For the terms of the last line in (F.15) that contain $G_{\mu/\nu,\lambda}(t)$, we use the partition (recall that $\mu < \frac{1}{2}$)

$$\nu \in [0,1] \;=\; \Big[0, \sqrt{\tfrac{1}{2}}\Big) \cup \Big[\sqrt{\tfrac{1}{2}}, \sqrt{\tfrac{1}{2}+\mu}\Big) \cup \Big[\sqrt{\tfrac{1}{2}+\mu}\,, 1\Big]\,,$$

so that

$$\begin{aligned}
&\int_0^1 \nu^{d-2} \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \int_0^\infty \big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big)\, G_{\mu/\nu,\lambda}(t)\, dt\, d\lambda\, d\nu \\
&\leqslant \int_0^1 \nu^{d-2} \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \lambda \wedge \lambda^{-1}\, d\lambda\, d\nu \;=\; \sum_{k=1}^4 I_\mu^{(k)}\,,
\end{aligned}$$

where

$$\begin{aligned}
I_\mu^{(1)} &:= \int_0^{\sqrt{\frac{1}{2}}} \nu^{d-2} \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \lambda^{-1}\, d\lambda\, d\nu\,, \qquad I_\mu^{(2)} := \int_{\sqrt{\frac{1}{2}}}^{\sqrt{\frac{1}{2}+\mu}} \nu^{d-2} \int_{\sqrt{\frac{1}{\nu^2}-1}}^{1} \lambda\, d\lambda\, d\nu\,, \\
I_\mu^{(3)} &:= \int_{\sqrt{\frac{1}{2}}}^{\sqrt{\frac{1}{2}+\mu}} \nu^{d-2} \int_1^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \lambda^{-1}\, d\lambda\, d\nu\,, \quad I_\mu^{(4)} := \int_{\sqrt{\frac{1}{2}+\mu}}^{1} \nu^{d-2} \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \lambda\, d\lambda\, d\nu\,.
\end{aligned}$$

We have

$$\begin{aligned}
I_\mu^{(1)} &= \tfrac{1}{2} \int_0^{\sqrt{\frac{1}{2}}} \nu^{d-2} \ln\Big(1 + \tfrac{2\mu}{1-\nu^2}\Big) d\nu \;\leqslant\; \mu \int_0^{\sqrt{\frac{1}{2}}} \tfrac{1}{1-\nu^2}\, d\nu \;=\; C\,\mu\,, \\
I_\mu^{(2)} &= \tfrac{1}{2} \int_{\sqrt{\frac{1}{2}}}^{\sqrt{\frac{1}{2}+\mu}} \nu^{d-2} \Big(2 - \tfrac{1}{\nu^2}\Big) d\nu \;\leqslant\; \sqrt{\tfrac{1}{2}+\mu} - \sqrt{\tfrac{1}{2}} \;\leqslant\; \mu\,, \\
I_\mu^{(3)} &= \tfrac{1}{2} \int_{\sqrt{\frac{1}{2}}}^{\sqrt{\frac{1}{2}+\mu}} \nu^{d-2} \ln\Big(\tfrac{1+2\mu}{\nu^2} - 1\Big) d\nu \;\leqslant\; \sqrt{\tfrac{1}{2}+\mu} - \sqrt{\tfrac{1}{2}} \;\leqslant\; \mu\,, \\
I_\mu^{(4)} &= \mu \int_{\sqrt{\frac{1}{2}+\mu}}^1 \nu^{d-4}\, d\nu \;\leqslant\; \mu \int_{\sqrt{\frac{1}{2}}}^1 \nu^{d-4}\, d\nu \;=\; C\,\mu\,.
\end{aligned}$$

Therefore, we conclude that, by (F.15),

$$\int_0^\infty \nu^{d-2} \int_0^\infty \int_0^\infty \big|\big(\nu\,\psi_{\mu/\nu}(\lambda^2+1)-1\big)_- - \big(\nu\,\psi_0(\lambda^2+1)-1\big)_-\big|\, G_{\mu/\nu,\lambda}(t)\, dt\, d\lambda\, d\nu \;\leqslant\; C\,\mu\,. \quad \text{(F.16)}$$

It remains to study the terms in (F.15) that contain $\cos(2\beta_{\mu/\nu,\lambda}(t))$. As above, we consider the integrals in t separately in the regions where $t \in [0,\nu)$, $t \in [\nu, 1)$, and $t \in [1,\infty)$. First, we have

$$\begin{aligned}
&\int_0^1 \nu^{d-1} \int_0^\nu \bigg| \int_0^{\sqrt{\frac{1}{\nu^2}-1}} \big(\psi_0(\lambda^2+1) - \psi_{\mu/\nu}(\lambda^2+1)\big)\, \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda \bigg|\, dt\, d\nu \\
&\leqslant \int_0^1 \nu^{d-1} \int_0^\nu \int_0^{1/\nu} \big|\psi_0(\lambda^2+1) - \psi_{\mu/\nu}(\lambda^2+1)\big|\, d\lambda\, dt\, d\nu \;\leqslant\; \mu \int_0^1 \nu^{d-2}\, d\nu \;\leqslant\; \mu\,,
\end{aligned}$$

as well as

$$\int_1^{\sqrt{1+2\mu}} \nu^{d-2} \int_0^{\nu} \left| \int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big)\, \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda \right| dt\, d\nu$$

$$\leqslant \int_1^{\sqrt{1+2\mu}} \nu^{d-2} \sqrt{1+2\mu-\nu^2}\; d\nu \;\leqslant\; \sqrt{2\mu}\,\big(\sqrt{1+2\mu}-1\big) \;\leqslant\; 2\mu\,,$$

and

$$\int_0^1 \nu^{d-2} \int_0^{\nu} \left| \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big)\, \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda \right| dt\, d\nu$$

$$\leqslant \int_0^1 \nu^{d-2} \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \big(1+\mu-\sqrt{1+\mu^2}\big)\, d\lambda\, d\nu$$

$$\leqslant \int_0^1 \nu^{d-2} \big(\sqrt{2\mu+1-\nu^2}-\sqrt{1-\nu^2}\big)\big(\sqrt{2\mu+1+\mu^2}-\sqrt{1+\mu^2}\big)\, d\nu \;\leqslant\; 2\mu\,.$$

In the region where $t\in[\nu,1)$, by integrating by parts, we obtain for the first term in (F.15),

$$\int_0^1 \nu^{d-1} \int_{\nu}^1 \left| \int_0^{\sqrt{\frac{1}{\nu^2}-1}} \big(\psi_0(\lambda^2+1)-\psi_{\mu/\nu}(\lambda^2+1)\big)\, \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda \right| dt\, d\nu$$

$$= \int_0^1 \nu^{d-1} \int_{\nu}^1 \frac{1}{2t} \Bigg| \big(\psi_0(\nu^{-2})-\psi_{\mu/\nu}(\nu^{-2})\big)\, \sin\big(2\beta_{\mu/\nu,\sqrt{\frac{1}{\nu^2}-1}}(t)\big)$$

$$- \int_0^{\sqrt{\frac{1}{\nu^2}-1}} \Big(\frac{\lambda}{\sqrt{\lambda^2+1}}-\frac{\lambda}{\sqrt{\lambda^2+1+\mu^2/\nu^2}}\Big)\, \sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda$$

$$- \int_0^{\sqrt{\frac{1}{\nu^2}-1}} \big(\psi_0(\lambda^2+1)-\psi_{\mu/\nu}(\lambda^2+1)\big)\, \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big) \frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\, d\lambda \Bigg| dt\, d\nu$$

$$\leqslant \mu \int_0^1 |\ln(\nu)|\, d\nu + \mu^{\delta} \int_0^1 \nu^{-\delta} |\ln(\nu)|\, d\nu + \mu \int_0^1 \big(2|\ln(\nu)|+|\ln(\nu)|^2\big)\, d\nu \;\leqslant C_\delta\, \mu^{\delta}\,,$$

since for all $\omega\geqslant 0$,

$$\frac{\partial}{\partial\omega}\frac{\lambda}{\sqrt{\lambda^2+1+\omega^2}} \;=\; \frac{\lambda\,\omega}{(\lambda^2+1+\omega^2)^{3/2}} \;\leqslant\; \frac{\lambda}{\lambda^2+1}\,,$$

and therefore,

$$\frac{\lambda}{\sqrt{\lambda^2+1}} - \frac{\lambda}{\sqrt{\lambda^2+1+\omega^2}} \;\leqslant\; 1\wedge\omega\,.$$

Similarly, integrating by parts in the second term in (F.15) gives

$$\int_1^{\sqrt{1+2\mu}} \nu^{d-2} \int_{\nu}^1 \left| \int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big) \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda \right| dt\, d\nu$$

$$= \int_1^{\sqrt{1+2\mu}} \nu^{d-2} \int_{\nu}^1 \frac{1}{2t} \Bigg| \int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \frac{\nu\,\lambda}{\sqrt{\lambda^2+1+\mu^2/\nu^2}}\, \sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda$$

$$+ \int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big)\, \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big) \frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\, d\lambda \Bigg| dt\, d\nu$$

$$\leqslant \frac{\sqrt{2\mu}}{2} \int_1^{\sqrt{1+2\mu}} |\ln(\nu)|\, d\nu + \int_1^{\sqrt{1+2\mu}} |\ln(\nu)| \int_0^{\sqrt{2\mu}} 1\wedge\lambda^{-1}\, d\lambda\, d\nu \;\leqslant\; C\,\mu\,,$$

and for the third term in (F.15),

$$\begin{aligned}
&\int_0^1 \nu^{d-2} \int_\nu^1 \bigg| \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big) \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda \bigg|\, dt\, d\nu \\
&= \int_0^1 \nu^{d-2} \int_\nu^1 \frac{1}{2t} \bigg| \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \frac{\nu\,\lambda}{\sqrt{\lambda^2+1+\mu^2/\nu^2}} \sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda \\
&\quad + \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big) \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big) \frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\, d\lambda \bigg|\, dt\, d\nu \\
&\leqslant \frac{\mu}{2} \int_0^1 \nu^{d-2} |\ln(\nu)|\, d\nu + \big(1+\mu - \sqrt{1+\mu^2}\big) \int_0^1 \nu^{d-2} \big(\sqrt{2}+|\ln(\nu)|\big)\, d\nu \;\leqslant\; C\,\mu\,.
\end{aligned}$$

In the region where $t \in [1,\infty)$, integrating by parts in the sum of the terms in the first and the third lines of (F.15) that contain a factor of $\cos(2\beta_{\mu/\nu,\lambda}(t))$ gives

$$\begin{aligned}
&\int_1^\infty \int_0^1 \nu^{d-1} \int_0^{\sqrt{\frac{1}{\nu^2}-1}} \big(\psi_0(\lambda^2+1) - \psi_{\mu/\nu}(\lambda^2+1)\big) \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda\, dt\, d\nu \\
&+ \int_1^\infty \int_0^1 \nu^{d-2} \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big) \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda\, d\nu\, dt \\
&= -\int_1^\infty \frac{1}{2t} \int_0^1 \nu^{d-1} \bigg(\int_0^{\sqrt{\frac{1}{\nu^2}-1}} \Big(\tfrac{\lambda}{\sqrt{\lambda^2+1}} - \tfrac{\lambda}{\sqrt{\lambda^2+1+\mu^2/\nu^2}} \Big) \sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda \\
&\qquad - \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \frac{\lambda}{\sqrt{\lambda^2+1+\mu^2/\nu^2}} \sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda \bigg)\, d\nu\, dt \qquad \text{(F.17)} \\
&\quad - \int_1^\infty \frac{1}{t} \int_0^1 \nu^{d-2} \bigg(\int_0^{\sqrt{\frac{1}{\nu^2}-1}} \nu\big(\psi_0(\lambda^2+1) - \psi_{\mu/\nu}(\lambda^2+1)\big) \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big) \frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\, d\lambda \\
&\qquad + \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big) \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big) \frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\, d\lambda \bigg)\, d\nu\, dt\,, \qquad \text{(F.18)}
\end{aligned}$$

where the non-zero boundary terms cancel each other. After another integration by parts, (F.17) equals

$$\begin{aligned}
&-\int_1^\infty \frac{1}{4t^2} \int_0^1 \nu^{d-1} \bigg[\sqrt{1-\nu^2}\, \sin\big(2\beta_{\mu/\nu,\sqrt{\frac{1}{\nu^2}-1}}(t)\big) - \frac{\sqrt{1+2\mu-\nu^2}}{1+\mu} \sin\big(2\beta_{\mu/\nu,\sqrt{\frac{1+2\mu}{\nu^2}-1}}(t)\big) \\
&\quad - \int_0^{\sqrt{\frac{1}{\nu^2}-1}} \bigg(\tfrac{1}{\sqrt{\lambda^2+1}} \Big(1 - \tfrac{\lambda^2}{\lambda^2+1}\Big) - \tfrac{1}{\sqrt{\lambda^2+1+\mu^2/\nu^2}} \Big(1 - \tfrac{\lambda^2}{\lambda^2+1+\mu^2/\nu^2}\Big) \bigg) \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda \\
&\quad - 2 \int_0^{\sqrt{\frac{1}{\nu^2}-1}} \Big(\tfrac{\lambda}{\sqrt{\lambda^2+1}} - \tfrac{\lambda}{\sqrt{\lambda^2+1+\mu^2/\nu^2}} \Big) \sin\big(2\beta_{\mu/\nu,\lambda}(t)\big) \frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\, d\lambda \\
&\quad + \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \tfrac{1}{\sqrt{\lambda^2+1+\mu^2/\nu^2}} \Big(1 - \tfrac{\lambda^2}{\lambda^2+1+\mu^2/\nu^2}\Big) \cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\, d\lambda \\
&\quad + 2 \int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \frac{\lambda}{\sqrt{\lambda^2+1+\mu^2/\nu^2}} \sin\big(2\beta_{\mu/\nu,\lambda}(t)\big) \frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\, d\lambda \bigg]\, d\nu\, dt \;=:\; D_1(\mu)\,.
\end{aligned}$$

Since for all $\omega > 0$, by an explicit computation

$$\Big|\frac{\partial}{\partial\mu}\Big(\tfrac{\sqrt{1+2\mu-\nu^2}}{1+\mu}\,\sin\big(2\beta_{\omega,\sqrt{\frac{1+2\mu}{\nu^2}-1}}\big)\Big)\Big| \leqslant 1+t\,,$$

and therefore, for all $\delta\in(0,1)$,

$$\Big|\sqrt{1-\nu^2}\,\sin\big(2\beta_{\mu/\nu,\sqrt{\frac{1}{\nu^2}-1}}(t)\big)-\tfrac{\sqrt{1+2\mu-\nu^2}}{1+\mu}\,\sin\big(2\beta_{\mu/\nu,\sqrt{\frac{1+2\mu}{\nu^2}-1}}(t)\big)\Big| \leqslant 2\wedge(1+t)\mu \leqslant 2(1+t^\delta)\,\mu^\delta.$$

Moreover,

$$\Big|\frac{\partial}{\partial\omega}\Big(\tfrac{1}{\sqrt{\lambda^2+1+\omega^2}}\Big(1-\tfrac{\lambda^2}{\lambda^2+1+\omega^2}\Big)\Big)\Big| \leqslant \frac{4}{\lambda^2+1}\,,$$

and thus, for $\nu\in(0,1)$ and $\omega>0$,

$$\Big|\int_0^{\sqrt{\frac{1}{\nu^2}-1}}\Big(\tfrac{1}{\sqrt{\lambda^2+1}}\Big(1-\tfrac{\lambda^2}{\lambda^2+1}\Big)-\tfrac{1}{\sqrt{\lambda^2+1+\omega^2}}\Big(1-\tfrac{\lambda^2}{\lambda^2+1+\omega^2}\Big)\Big)\cos\big(2\beta_{\omega,\lambda}(t)\big)\,d\lambda\Big| \leqslant 4(2-\nu)\,\omega\,.$$

Also, since $\frac{\partial}{\partial\omega}\frac{\lambda}{\sqrt{\lambda^2+1+\omega^2}} = \frac{\lambda\,\omega}{(\lambda^2+1+\omega^2)^{3/2}} \leqslant \frac{1}{\sqrt{\lambda^2+1}}$ we have for all $\omega>0$,

$$\Big|\int_0^{\sqrt{\frac{1}{\nu^2}-1}}\Big(\tfrac{\lambda}{\sqrt{\lambda^2+1}}-\tfrac{\lambda}{\sqrt{\lambda^2+1+\omega^2}}\Big)\,\sin\big(2\beta_{\omega,\lambda}(t)\big)\,\frac{d\vartheta_\omega}{d\lambda}(\lambda)\,d\lambda\Big| \leqslant (2-\nu)\,\omega\,.$$

Since

$$\sqrt{1+2\mu-\nu^2}-\sqrt{1-\nu^2} \leqslant \sqrt{2\mu}\wedge\frac{2\mu}{\sqrt{1-\nu^2}} \leqslant (2\mu)^{\frac12+\frac{\delta}{2}}\,(1-\nu^2)^{\delta/2} \leqslant (2\mu)^\delta\,(1-\nu^2)^{\delta/2}\,,$$

for any $\delta\in(0,1)$, we have

$$\int_0^1\nu^{d-1}\Big|\int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}}\tfrac{1}{\sqrt{\lambda^2+1+\mu^2/\nu^2}}\Big(1-\tfrac{\lambda^2}{\lambda^2+1+\mu^2/\nu^2}\Big)\,\cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\,d\lambda\Big|\,d\nu \leqslant C_\delta\,\mu^\delta\,,$$

as well as

$$\int_0^1\nu^{d-1}\Big|\int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}}\tfrac{\lambda}{\sqrt{\lambda^2+1+\mu^2/\nu^2}}\,\sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)\,\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\,d\lambda\Big|\,d\nu \leqslant C_\delta\,\mu^\delta\,.$$

Combining the above estimates, we obtain

$$|D_1(\mu)| \leqslant \int_1^\infty\frac{1}{t^2}\int_0^1\nu^{d-2}(\nu\,\mu^\delta(1+t^\delta)+\mu)\,d\nu\,dt \leqslant C_\delta\,\mu^\delta$$

for any $\delta\in(0,1)$.

Similarly, another integration by parts in (F.18) gives

$$\begin{aligned}\int_1^\infty\frac{1}{4t^2}\int_0^1\nu^{d-2}\Big[\nu\int_0^{\sqrt{\frac{1}{\nu^2}-1}}&\frac{\partial}{\partial\lambda}\Big(\big(\psi_0(\lambda^2+1)-\psi_{\mu/\nu}(\lambda^2+1)\big)\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\Big)\sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)\,d\lambda\\ &+2\nu\int_0^{\sqrt{\frac{1}{\nu^2}-1}}\big(\psi_0(\lambda^2+1)-\psi_{\mu/\nu}(\lambda^2+1)\big)\Big(\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\Big)^2\cos\big(2\beta_{\mu/\nu}(t)\big)\,d\lambda\\ &+\int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}}\frac{\partial}{\partial\lambda}\Big(\big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big)\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\Big)\sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)\,d\lambda\\ &+2\int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}}\big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big)\Big(\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\Big)^2\cos\big(2\beta_{\mu/\nu}(t)\big)\,d\lambda\Big]\,d\nu\,dt =: D_2(\mu).\end{aligned}$$

By Lemma 18, we have

$$\left|\frac{\partial}{\partial\lambda}\Big(\big(\psi_0(\lambda^2{+}1)-\psi_\omega(\lambda^2{+}1)\big)\frac{d\vartheta_\omega}{d\lambda}(\lambda)\Big)\right| \leqslant \frac{4}{\pi}\,\frac{1\wedge\omega}{\lambda^2{+}1}$$

and

$$\left|\big(\psi_0(\lambda^2{+}1)-\psi_\omega(\lambda^2{+}1)\big)\Big(\frac{d\vartheta_\omega}{d\lambda}(\lambda)\Big)^2\right| \leqslant \frac{1}{\pi^2}\frac{1\wedge\omega}{\sqrt{\lambda^2{+}1}}\,,$$

and thus the first two terms in $D_2(\mu)$ are bounded by

$$\int_1^\infty \frac{1}{2t^2}\int_0^1 \nu^{d-1}\int_0^{\sqrt{\frac{1}{\nu^2}-1}} \frac{1\wedge\mu/\nu}{\sqrt{\lambda^2{+}1}} \leqslant \mu^\delta \int_0^1 \nu^{-\delta}\,d\nu \,=\, C_\delta\,\mu^\delta$$

for any $\delta\in(0,1)$. Moreover,

$$\begin{aligned}
&\left|\int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \frac{\partial}{\partial\lambda}\Big(\big(1{-}\nu\,\psi_{\mu/\nu}(\lambda^2{+}1)\big)\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\Big)\sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)\,d\lambda\right|\\
&\leqslant \frac{3}{\pi}\int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}}\Big(\frac{\nu\,\lambda}{(\lambda^2{+}1)^{3/2}}+\frac{\mu}{\lambda^2{+}1}\Big)\,d\lambda\\
&\leqslant \big(\sqrt{1{+}2\mu{-}\nu^2}-\sqrt{1{-}\nu^2}\big)+\mu\int_0^\infty\frac{1}{\lambda^2{+}1}\,d\lambda \leqslant C_\delta\,\mu^\delta\,(1{-}\nu^2)^{\delta/2}
\end{aligned}$$

for all $\nu\in(0,1)$, and

$$\left|\int_{\sqrt{\frac{1}{\nu^2}-1}}^{\sqrt{\frac{1+2\mu}{\nu^2}-1}}\big(1{-}\nu\,\psi_{\mu/\nu}(\lambda^2{+}1)\big)\Big(\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\Big)^2\cos\big(2\beta_{\mu/\nu}(t)\big)\,d\lambda\right| \leqslant \frac{1}{\pi^2}\int_0^\infty\frac{\mu}{\lambda^2{+}1}\,d\lambda \,=\, C\,\mu\,.$$

Combining the estimates, we obtain for any $\delta\in(0,1)$,

$$|D_2(\mu)| \leqslant C_\delta\,\mu^\delta\,.$$

It remains to integrate by parts in the term containing $\cos(2\beta_{\mu/\nu,\lambda}(t))$ in the second line of (F.15) in the region where $t\in[1,\infty)$, i.e.

$$\begin{aligned}
&\int_1^\infty\int_1^{\sqrt{1+2\mu}}\nu^{d-2}\int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}}\big(1{-}\nu\,\psi_{\mu/\nu}(\lambda^2{+}1)\big)\cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\,d\lambda\,d\nu\,dt\\
&= -\int_1^\infty\frac{1}{2t}\int_1^{\sqrt{1+2\mu}}\nu^{d-2}\Big[\int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}}\frac{\nu\,\lambda}{\sqrt{\lambda^2{+}1{+}\mu^2/\nu^2}}\,\sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)\,d\lambda\\
&\qquad+\int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}}\big(1{-}\nu\,\psi_{\mu/\nu}(\lambda^2{+}1)\big)\,\cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\,d\lambda\Big]\,d\nu\,dt\,. \qquad (F.19)
\end{aligned}$$

After another integration by parts, the first term in (F.19) equals

$$\begin{aligned}
&-\int_1^\infty\frac{1}{4t^2}\int_1^{\sqrt{1+2\mu}}\nu^{d-1}\Big[-\frac{\sqrt{1{+}2\mu{-}\nu^2}}{1{+}\mu}\,\cos\Big(2\beta_{\mu/\nu,\sqrt{\frac{1+2\mu}{\nu^2}-1}}(t)\Big)\\
&\qquad+\int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}}\frac{(1{+}\mu^2/\nu^2)}{(\lambda^2{+}1{+}\mu^2/\nu^2)^{3/2}}\,\cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\,d\lambda\\
&\qquad-2\int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}}\frac{\lambda}{\sqrt{\lambda^2{+}1{+}\mu^2/\nu^2}}\,\sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)\,\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\,d\lambda\Big]\,d\nu\,dt \,=:\, D_3(\mu)\,.
\end{aligned}$$

Since $\sqrt{1+2\mu}-1 \leqslant \mu$, it follows that

$$|D_3(\mu)| \leqslant \int_1^\infty \frac{1}{t^2}\int_1^{\sqrt{1+2\mu}} \nu^{d-1}(1+\nu)\,d\nu \leqslant C\,\mu\,.$$

Similarly, for the second term in (F.19), we obtain

$$\begin{aligned}
-\int_1^\infty \frac{1}{4t^2}\int_1^{\sqrt{1+2\mu}} \nu^{d-2}\Big[-\int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \frac{\nu\,\lambda}{\sqrt{\lambda^2+1+\mu^2/\nu^2}}\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)\,d\lambda \\
-\int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big)\frac{d^2\vartheta_{\mu/\nu}}{d\lambda^2}(\lambda)\sin\big(2\beta_{\mu/\nu,\lambda}(t)\big)\,d\lambda \\
-2\int_0^{\sqrt{\frac{1+2\mu}{\nu^2}-1}} \big(1-\nu\,\psi_{\mu/\nu}(\lambda^2+1)\big)\Big(\frac{d\vartheta_{\mu/\nu}}{d\lambda}(\lambda)\Big)^2\cos\big(2\beta_{\mu/\nu,\lambda}(t)\big)\,d\lambda\Big]\,d\nu\,dt =: D_4(\mu)\,,
\end{aligned}$$

and therefore, as for $D_3(\mu)$,

$$|D_4(\mu)| \leqslant \int_1^\infty \frac{1}{t^2}\int_1^{\sqrt{1+2\mu}} \nu^{d-2}(\nu+1)\,d\nu \leqslant C\,\mu\,.$$

Finally, by (F.15),

$$\Big|\int_0^\infty\!\!\int_{\mathbb{R}^{d-1}} \mathcal{I}^{(1)}_{\mu/|\xi'|}(|\xi'|,t)\,d\xi'\,dt\Big| \leqslant C_\delta\,\mu^\delta$$

for any $\delta \in (0,1)$. Hence, together with (F.13) and (F.3), this proves the claim. □

F.2. **Proof of** (6.16)**.** Here we prove that the integral in the bound for $R_{\mu,h}(\phi)$ in the proof of Lemma 24 is uniformly bounded in μ and h. More precisely, we prove that for any $\sigma \in (0,\frac12)$ there exists a constant $C_\sigma > 0$ such that, for all $\nu > 0$,

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \Big|(-\Delta_{x'})^\sigma\Big(\big(\phi(x)-\phi(y)\big)^2\theta_\nu(|x-y|)\Big)\Big|\,dx\,dy \leqslant C_\sigma\,. \tag{6.16}$$

Proof. By translation, we can assume that ϕ is supported in the unit ball around 0. By the massless analogue [3] of the integral representation (0.10), there exists $C>0$ such that, for all $f \in C^1 \cap L^\infty(\mathbb{R}^{d-1})$,

$$(-\Delta)^\sigma f(x') = C\int_{\mathbb{R}^{d-1}} \frac{f(x')-f(z')}{|x'-z'|^{d-1+2\sigma}}\,dy'$$

for almost every $x' \in \mathbb{R}^{d-1}$. Note that for the general case of $0<\sigma<1$, due to the singularity at $y'=x'$, the integral on the right side is not defined, but rather has to be replaced by the principle value of the integral over $|x'-y'|>\varepsilon$ for $\varepsilon \to 0^+$. However, in the case of $0<\sigma<\frac12$ we have

$$\begin{aligned}
\int_{\mathbb{R}^{d-1}} \frac{|f(x')-f(z')|}{|x'-z'|^{d-1+2\sigma}}\,dz' &\leqslant \int_{|x'-z'|\leqslant R} \frac{\|f'\|_\infty|x'-z'|}{|x'-z'|^{d-1+2\sigma}} + \int_{|x'-z'|>R} \frac{2\|f\|_\infty}{|x'-z'|^{d-1+2\sigma}} \\
&\leqslant C\left(\int_0^R t^{-2\sigma}dt + \int_R^\infty t^{-2\sigma-1}dt\right) < \infty\,.
\end{aligned}$$

Hence, for $f_{x_d,y}(x') := (\phi(x)^2-\phi(y))^2\theta_\nu(|x-y|)$, we obtain

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \big|(-\Delta_{x'})^\sigma f_{x_d,y}(x')\big|\,dx\,dy \leqslant C\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^{d-1}} \frac{|f_{x_d,y}(x')-f_{x_d,y}(z')|}{|x'-z'|^{d-1+2\sigma}}\,dz'\,dx\,dy\,. \tag{F.20}$$

In the following, we find upper bounds for the right sight of (F.20), where the integration in x and y is restricted to the regions (i) $B_1{\times}B_1$, (ii) $(\mathbb{R}^d\backslash B_1){\times}(\mathbb{R}^d\backslash B_1)$, (iii) $B_1{\times}(\mathbb{R}^d\backslash B_1)$, and (iv) $(\mathbb{R}^d\backslash B_1){\times}B_1$.

(i) In the region, where $(x,y)\in B_1{\times}B_1$, we have

$$\int_{B_1}\int_{B_1}\big|(-\Delta_{x'})^\sigma f_{x_d,y}(x')\big|\,dx\,dy \;\leqslant\; C\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{|x'-z'|<|x-y|/2}\frac{|f_{x_d,y}(x')-f_{x_d,y}(z')|}{|x'-z'|^{d-1+2\sigma}}\,dz'\,dx\,dy + C\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{|x'-z'|\geqslant|x-y|/2}\frac{|f_{x_d,y}(x')-f_{x_d,y}(z')|}{|x'-z'|^{d-1+2\sigma}}\,dz'\,dx\,dy\,.$$

First, for $|x'-z'|<|x-y|/2$ we will prove that for any $\tau\in(0,1)$ there exists $C>0$ such that

$$\big|f_{x_d,y}(z')-f_{x_d,y}(x')\big| \;\leqslant\; C\,|x'-z'|^\beta\,|x-y|^{-d+1-\beta}\,. \tag{F.21}$$

For this, we write

$$f_{x_d,y}(z')-f_{x_d,y}(x') \;=\; \sum_{j=1}^{d-1}\frac{z_j-x_j}{|z'-x'|}\int_0^{|z'-x'|}\big(\partial_j f_{x_d,y}\big)\left(x'+t\frac{z'-x'}{|z'-x'|}\right)dt\,, \tag{F.22}$$

where for $j\in\{1,\ldots,n-1\}$,

$$\partial_j f_{x_d,y}(x') \;=\; 2(\phi(x)-\phi(y))\,\partial_j\phi(x)\,\theta_\nu(|x-y|)+(\phi(x)-\phi(y))^2\,\theta_\nu'(|x-y|)\,\frac{x_j-y_j}{|x-y|}\,.$$

Since, for all $\beta\in\mathbb{R}$, we have $K_\beta'(x)=\frac{\beta}{x}K_\beta(x)-K_{\beta+1}(x)$, and $K_{(d+1)/2}(t)\leqslant C\,t^{-(d+1)/2}$ (see Appendix D.2), it follows that $\theta'(t)=-(2\pi t)^{-(d+1)/2}K_{(d+3)/2}(t)$ and

$$|\theta_\nu'(t)| \;=\; \nu^{d+2}|\theta'(\nu t)| \;=\; \nu^{d+2}(2\pi\nu t)^{-(d+1)/2}K_{(d+3)/2}(\nu t) \;\leqslant\; C\,t^{-d-2}\,.$$

Together with $\theta_\nu(t)\leqslant C\,t^{-(d+1)}$, we obtain for all $j=0,\ldots,d{-}1$ that

$$|\partial_j f_{x_d,y}(x')| \;\leqslant\; C\|\nabla\phi\|_\infty^2\,|x-y|^{-d}\,. \tag{F.23}$$

Hence, by (F.22)

$$|f_{x_d,y}(z')-f_{x_d,y}(x')| \;\leqslant\; C\int_0^{|x'-z'|}\left(\left|x'+t\frac{z'-x'}{|z'-x'|}-y'\right|^2+(x_d-y_d)^2\right)^{-d/2}dt\,.$$

We have

$$\left|x'+t\frac{z'-x'}{|z'-x'|}-y'\right|^2+(x_d-y_d)^2 \;=\; |x-y|^2+t^2+2t\frac{(x'-y')(z'-x')}{|z'-x'|} \;\geqslant\; (|x-y|-t)^2\,,$$

and therefore, by Hölder's inequality, we obtain for any $\tau\in(0,1)$ that

$$\begin{aligned}|f_{x_d,y}(x')-f_{x_d,y}(z')| \;&\leqslant\; C\,|x'-z'|^\tau\left(\int_0^{|x'-z'|}\big(|x-y|-t\big)^{-d/(1-\tau)}dt\right)^{1-\tau}\\ &\leqslant\; C\,|x'-z'|^\tau\,|x-y|^{-d+1-\tau}\,,\end{aligned} \tag{F.24}$$

where in the second inequality we used the assumption $|x'-z'| < |x-y|/2$. This proves (F.21). It follows for $\tau \in (2\sigma, 1)$ that

$$\begin{aligned}
&\int_{B_1}\int_{B_1}\int_{|x'-z'|\leqslant|x-y|/2} \frac{|f_{x_d,y}(x')-f_{x_d,y}(z')|}{|x'-z'|^{d-1+2\sigma}}\,dz'\;dx\,dy \\
&\leqslant\; C\int_{B_1}\int_{B_1}\int_{|x'-z'|\leqslant|x-y|/2} |x'-z'|^{-d+1+\tau-2\sigma}\,dz'\,|x-y|^{-d+1+\tau}\,dx\,dy \\
&=\; C\int_{B_1}\int_{B_1}\int_0^{|x-y|/2} t^{-1+\tau-2\sigma}\,dt\,|x-y|^{-d+1+\tau}\,dx\,dy \\
&=\; C\int_{B_1}\int_{B_1} |x-y|^{-d+1+2\tau-2\sigma}\,dx\,dy \\
&\leqslant\; C\int_0^2 t^{2\tau-2\sigma}\,dt \;=\; C_\sigma\,.
\end{aligned} \tag{F.25}$$

Next, in the case $|x'-z'| > |x-y|/2$,

$$\left|f_{x_d,y}(x')-f_{x_d,y}(z')\right| \;\leqslant\; f_{x_d,y}(x')+f_{x_d,y}(z')\,. \tag{F.26}$$

We are going to find bounds for the resulting integrals separately. First, since

$$f_{x_d,y}(x') \;\leqslant\; C\,|x-y|^{-d+1} \tag{F.27}$$

and

$$\int_{|x'-z'|>|x-y|/2} |x'-z'|^{-d+1-2\sigma}\,dz' \;=\; |\mathbb{S}^{d-2}|\int_{|x-y|/2}^\infty t^{-1-2\sigma}\,dt \;=\; C_\sigma\,|x-y|^{-2\sigma},$$

it follows that

$$\begin{aligned}
&\int_{B_1}\int_{B_1}\int_{|x'-z'|>|x-y|/2} \frac{f_{x_d,y}(x')}{|x'-z'|^{d-1+2\sigma}}\,dz'\,dx\,dy \\
&\leqslant\; C_\sigma\int_{B_1}\int_{B_1} |x-y|^{-d+1-2\sigma}\,dx\,dy \;\leqslant\; C_\sigma\int_0^2 t^{-2\sigma}\,dt \;=\; C_\sigma\,.
\end{aligned} \tag{F.28}$$

For the second term in (F.26), let $p > (d-1)/(2\sigma)$ and let q be its Hölder conjugate (note that $p>1$, since $d\leqslant 2$ and $2\sigma<1$). We have

$$\int_{|x'-z'|>|x-y|/2} |x'-z'|^{(-d+1-2\sigma)p}\,dz' \;=\; C_\sigma\,|x-y|^{(-d+1-2\sigma)p+d-1}\,.$$

Moreover, by (F.27)

$$\begin{aligned}
\int_{|x'-z'|>|x-y|/2} f_{x_d,y}(z')^q\,dz' \;&\leqslant\; C\int_{\mathbb{R}^{d-1}} \left(|z'-y'|^2+(x_d-y_d)^2\right)^{(-d+1)q/2}\,dz' \\
&=\; C\,|x_d-y_d|^{(-d+1)q+d-1}\,,
\end{aligned}$$

since

$$\int_{\mathbb{R}^{d-1}} (|z'|^2+c^2)^{(-d+1)q/2}\,dz' \;=\; c^{(-d+1)q+d-1}\,|\mathbb{S}^{d-2}|\int_0^\infty \frac{s^{d-2}}{(s^2+1)^{(d-1)q/2}}\,ds \;<\; \infty$$

for any $c>0$. Hence by Hölder's inequality

$$\int_{|x'-z'|>|x-y|/2} \frac{f_{x_d,y}(z')}{|x'-z'|^{d-1+2\sigma}}\,dz' \leqslant C_\sigma\;|x-y|^{-d+1-2\sigma+(d-1)/p}\,|x_d-y_d|^{-d+1+(d-1)/q}\,.$$

It follows that

$$\begin{aligned}
&\int_{B_1}\int_{B_1}\int_{|x'-z'|>|x-y|/2} \frac{f_{x_d,y}(z')}{|x'-z'|^{d-1+2\sigma}}\,dz'\,dx\,dy \\
&\leqslant\ C_\sigma \int_{B_2} |x|^{-d+1-2\sigma+(d-1)/p}\,|x_d|^{-d+1+(d-1)/q}\,dx \\
&\leqslant\ C_\sigma \int_0^2 t^{-d+1+(d-1)/q} \int_0^2 s^{d-2}(s^2+t^2)^{(-d+1)/2-\sigma+(d-1)/(2p)} ds\,dt \\
&=\ C_\sigma \int_0^2 t^{-d+1+(d-1)(1/q+1/p)-2\sigma} dt \int_0^2 \frac{s^{d-2}}{(s^2+1)^{(d-1)/2+\sigma-(d-1)/(2p)}}\,ds \\
&=\ C_\sigma \int_0^2 t^{-2\sigma} dt\ =\ C_\sigma\ . \qquad \text{(F.29)}
\end{aligned}$$

Hence, by (F.28) and (F.29), we have

$$\int_{B_1}\int_{B_1}\int_{|x'-z'|>|x-y|/2} \frac{|f_{x_d,y}(z')-f_{x_d,y}(x')|}{|x'-z'|^{d-1+2\sigma}}\,dz' dx\,dy\ \leqslant\ C_\sigma\ . \qquad \text{(F.30)}$$

The estimates (F.25) and (F.30) prove that, for any $\sigma\in(0,1/2)$, there exists $C_\sigma>0$ such that

$$\int_{B_1}\int_{B_1}\int_{\mathbb{R}^{d-1}} \frac{|f_{x_d,y}(z')-f_{x_d,y}(x')|}{|x'-z'|^{d-1+2\sigma}}\,dz' dx\,dy\ \leqslant\ C_\sigma\ . \qquad \text{(F.31)}$$

(ii) For the integral over $\mathbb{R}^d\backslash B_1\times\mathbb{R}^d\backslash B_1$, since $\operatorname{supp}\phi\subset B_1$, we have

$$\begin{aligned}
&\int_{\mathbb{R}^d\backslash B_1}\int_{\mathbb{R}^d\backslash B_1}\int_{\mathbb{R}^{d-1}} \frac{|f_{x_d,y}(z')-f_{x_d,y}(x')|}{|x'-z'|^{d-1+2\sigma}}\,dz' dx\,dy \\
&= \int_{\mathbb{R}^d\backslash B_1}\int_{\mathbb{R}^d\backslash B_1}\int_{\mathbb{R}^{d-1}} \frac{\phi(z',x_d)^2}{|x'-z'|^{d-1+2\sigma}}\,\theta_m(|(z',x_d)-y|)\,dz' dx\,dy \\
&= \int_{|\zeta|\leqslant 1}\int_{|x'|^2>1-\zeta_d^2}\int_{|y|>1} \frac{\phi(\zeta)^2}{|x'-\zeta'|^{d-1+2\sigma}}\,\theta_m(|\zeta-y|)\,dy\,dx' d\zeta\,, \qquad \text{(F.32)}
\end{aligned}$$

where we have set $\zeta:=(z',x_d)$. We split the x'-integration into $|x'-\zeta|\leqslant 1$ and $|x'-\zeta|>1$. In the first region, we also split the y-integration into $|\zeta-y|>|x'-\zeta'|$ and $|\zeta-y|\leqslant|x'-\zeta'|$. Since for $|y|>1$ and $|x'|^2+\zeta_d^2>1$ we have $\phi(y)=0=\phi(x',\zeta_d)$, it follows that

$$\begin{aligned}
&\int_{|x'|^2>1-\zeta_d^2,|x'-\zeta'|\leqslant 1}\int_{|y|>1} \frac{\phi(\zeta)^2}{|x'-\zeta'|^{d-1+2\sigma}}\,\theta_m(|\zeta-y|)\,dy\,dx' \\
&\leqslant C\int_{|x'|^2>1-\zeta_d^2,|x'-\zeta'|\leqslant 1} \frac{1}{|x'-\zeta'|^{d-1+2\sigma}}\,\times \\
&\quad\times\left(\int_{|y|>1,|\zeta-y|>|x'-\zeta'|} \frac{(\phi(x',\zeta_d)-\phi(\zeta))^2}{|\zeta-y|^{d+1}}\,dy + \int_{|y|>1,|\zeta-y|\leqslant|x'-\zeta'|} \frac{(\phi(\zeta)-\phi(y))^2}{|\zeta-y|^{d+1}}\,dy\right) dx' \\
&\leqslant C\int_{|x'|^2>1-\zeta_d^2,|x'-\zeta'|\leqslant 1} \frac{1}{|x'-\zeta'|^{d-1+2\sigma}}\left(|x'-\zeta'|^2\int_{|x'-\zeta'|}^\infty t^{-2}\,dt + \int_0^{|x'-\zeta'|} dt\right) dx' \\
&\leqslant C\int_{|x'-\zeta'|\leqslant 1} \frac{1}{|x'-\zeta'|^{d-2+2\sigma}}\,dx'\ =\ C\int_0^1 t^{-2\sigma} dt\ =\ C_\sigma\ . \qquad \text{(F.33)}
\end{aligned}$$

For the integral over $|x'-\zeta| > 1$, it suffices to split the y-integration into $|\zeta-y| > 1$ and $|\zeta-y| \leqslant 1$. We find

$$\begin{aligned}
&\int_{|x'|^2>1-\zeta_d^2, |x'-\zeta'|>1} \int_{|y|>1} \frac{\phi(\zeta)^2}{|x'-\zeta'|^{d-1+2\sigma}}\, \theta_m(|\zeta-y|)\, dy\, dx' \\
&\leqslant C \int_{|x'|^2>1-\zeta_d^2, |x'-\zeta'|>1} \frac{1}{|x'-\zeta'|^{d-1+2\sigma}} \times \\
&\quad \times \left(\int_{|y|>1, |\zeta-y|>1} \frac{1}{|\zeta-y|^{d+1}}\, dy + \int_{|y|>1, |\zeta-y|\leqslant 1} \frac{(\phi(\zeta)-\phi(y))^2}{|\zeta-y|^{d+1}}\, dy \right) dx' \\
&\leqslant C \int_{|x'-\zeta'|>1} \frac{1}{|x'-\zeta'|^{d-1+2\sigma}} \left(\int_1^\infty t^{-2}\, dt + \int_0^1 dt \right) dx' \\
&= C \int_1^\infty t^{-1-2\sigma} dt \;=\; C_\sigma\,. \qquad \text{(F.34)}
\end{aligned}$$

Hence, by (F.32),(F.33) and (F.34), for each $\sigma \in (0, 1/2)$ there exists $C_\sigma > 0$ such that

$$\int_{\mathbb{R}^d\setminus B_1} \int_{\mathbb{R}^d\setminus B_1} \int_{\mathbb{R}^{d-1}} \frac{|f_{x_d,y}(z') - f_{x_d,y}(x')|}{|x'-z'|^{d-1+2\sigma}}\, dz' dx\, dy \;\leqslant\; C\,. \qquad \text{(F.35)}$$

(iii) For the integral over $(x, y) \in B_1 \times \mathbb{R}^d\setminus B_1$, we have

$$\begin{aligned}
&\int_{\mathbb{R}^d\setminus B_1} \int_{B_1} \int_{\mathbb{R}^{d-1}} \frac{|f_{x_d,y}(z') - f_{x_d,y}(x')|}{|x'-z'|^{d-1+2\sigma}}\, dz' dx\, dy \qquad \text{(F.36)} \\
&\leqslant C \int_{|x|\leqslant 1} \int_{|y|>1} \int_{\mathbb{R}^{d-1}} \frac{1}{|x'-z'|^{d-1+2\sigma}} \left| \frac{\phi(x)^2}{|x-y|^{d+1}} - \frac{\phi(z', x_d)^2}{|(z', x_d)-y|^{d+1}} \right| dz' dy\, dx\,,
\end{aligned}$$

since supp $\phi \subset B_1$. We don't have to treat the case where $|x-y| \leqslant r$ for any $r > 0$, since then $|y| \leqslant 1+r$ and therefore everything works as in the region $B_1 \times B_1$. Thus, we may assume that $|x-y| > 2$. For the integral over $\mathbb{R}^{d-1}$ where $|x'-z'| > 1$, we have

$$\begin{aligned}
&\int_{|x|\leqslant 1} \int_{|y|>1, |x-y|>2} \int_{|x'-z'|>1} \frac{\phi(x)^2}{|x'-z'|^{d-1+2\sigma} |x-y|^{d+1}}\, dz' dy\, dx \\
&\leqslant\; C \int_{|x|\leqslant 1} \int_{|x-y|>2} \frac{1}{|x-y|^{d+1}}\, dy\, dx \int_1^\infty t^{-1-2\sigma}\, dt \;=\; C_\sigma \int_2^\infty s^{-2} ds \;=\; C_\sigma\,,
\end{aligned}$$

and

$$\begin{aligned}
&\int_{|x|\leqslant 1} \int_{|y|>1} \int_{|x'-z'|>1} \frac{\phi(z', x_d)^2}{|x'-z'|^{d-1+2\sigma} |(z', x_d)-y|^{d+1}}\, dz' dy\, dx \\
&\leqslant\; \int_{|x|\leqslant 1} \int_{|x'-z'|>1} \frac{1}{|x'-z'|^{d-1+2\sigma}} \int_{|y|>1, |(z',x_d)-y|\leqslant 1} \frac{(\phi(z', x_d)-\phi(y))^2}{|(z', x_d)-y|^{d+1}}\, dy\, dz' dx \\
&\quad + C \int_{|x|\leqslant 1} \int_{|x'-z'|>1} \frac{1}{|x'-z'|^{d-1+2\sigma}} \int_{|(z',x_d)-y|>1} \frac{1}{|(z', x_d)-y|^{d+1}}\, dy\, dz' dx \\
&\leqslant\; C \int_{|x|\leqslant 1} \int_{|x'-z'|>1} \frac{1}{|x'-z'|^{d-1+2\sigma}}\, dz' dx \left(\int_0^1 dt + \int_1^\infty t^{-2}\, dt \right) \\
&\leqslant\; C \int_1^\infty t^{-1-2\sigma}\, dt \;=\; C_\sigma\,.
\end{aligned}$$

Hence, it follows that

$$\int_{|x|\leqslant 1}\int_{|y|>1}\int_{|x'-z'|>1}\frac{1}{|x'-z'|^{d-1+2\sigma}}\left|\frac{\phi(x)^2}{|x-y|^{d+1}}-\frac{\phi(z',x_d)^2}{|(z',x_d)-y|^{d+1}}\right|dz'dy\,dx\;\leqslant\;C_\sigma. \quad (F.37)$$

In the region where $|x'-z'|\leqslant 1$, we write

$$\begin{aligned}&\int_{|x|\leqslant 1}\int_{|y|>1,|x-y|>2}\int_{|x'-z'|\leqslant 1}\frac{1}{|x'-z'|^{d-1+2\sigma}}\left|\frac{\phi(x)^2}{|x-y|^{d+1}}-\frac{\phi(z',x_d)^2}{|(z',x_d)-y|^{d+1}}\right|dz'dy\,dx\\ &\leqslant\int_{|x|\leqslant 1}\int_{|x-y|>2}\int_{|x'-z'|\leqslant 1}\frac{|\phi(x)^2-\phi(z',x_d)^2|}{|x-y|^{d+1}|x'-z'|^{d-1+2\sigma}}\,dz'dy\,dx\\ &\quad+\int_{|x|\leqslant 1}\int_{|y|>1,|x-y|>2}\int_{|x'-z'|\leqslant 1}\frac{\phi(z',x_d)^2}{|x'-z'|^{d-1+2\sigma}}\left|\frac{1}{|x-y|^{d+1}}-\frac{1}{|(z',x_d)-y|^{d+1}}\right|dz'dy\,dx\,.\end{aligned}$$

For the first integral on the right side, we obtain

$$\int_{|x|\leqslant 1}\int_{|x-y|>2}\int_{|x'-z'|\leqslant 1}\frac{|\phi(x)^2-\phi(z',x_d)^2|}{|x-y|^{d+1}|x'-z'|^{d-1+2\sigma}}\,dz'dy\,dx\;\leqslant C\int_2^\infty t^{-2}dt\int_0^1 s^{-2\sigma}ds\;=\;C_\sigma\,.$$

For the second integral, by the same argument that leads to (F.24), we obtain for any $\tau\in(0,1)$,

$$\left|\frac{1}{|x-y|^{d+1}}-\frac{1}{|(z',x_d)-y|^{d+1}}\right|\;\leqslant\;C\,|x'-z'|^{\tau}\,|x-y|^{-d-1-\tau}\,,$$

since $|x'-z'|\leqslant 1<|x-y|/2$. This is the reason for the choice of $r=2$. Hence, for $\tau\in(2\sigma,1)$,

$$\begin{aligned}&\int_{|x|\leqslant 1}\int_{|y|>1,|x-y|>2}\int_{|x'-z'|\leqslant 1}\frac{\phi(z',x_d)^2}{|x'-z'|^{d-1+2\sigma}}\left|\frac{1}{|x-y|^{d+1}}-\frac{1}{|(z',x_d)-y|^{d+1}}\right|dz'dy\,dx\\ &\leqslant\;C\int_{|x|\leqslant 1}\int_{|x-y|>2}\frac{1}{|x-y|^{d+1+\tau}}\,dy\int_{|x'-z'|\leqslant 1}\frac{1}{|x'-z'|^{d-1-(\tau-2\sigma)}}\,dz'\,dx\\ &=\;C\int_2^\infty t^{-2-\tau}\,dt\int_0^1 s^{-1+\tau-2\sigma}\,ds\;=\;C_\sigma\,.\end{aligned}$$

Therefore,

$$\int_{|x|\leqslant 1}\int_{|y|>1}\int_{|x'-z'|\leqslant 1}\frac{1}{|x'-z'|^{d-1+2\sigma}}\left|\frac{\phi(x)^2}{|x-y|^{d+1}}-\frac{\phi(z',x_d)^2}{|(z',x_d)-y|^{d+1}}\right|dz'dy\,dx\;\leqslant\;C_\sigma. \quad (F.38)$$

By combining (F.37), (F.38), and (F.36) we obtain

$$\int_{\mathbb{R}^d\setminus B_1}\int_{B_1}\int_{\mathbb{R}^{d-1}}\frac{|f_{x_d,y}(z')-f_{x_d,y}(x')|}{|x'-z'|^{d-1+2\sigma}}\,dz'dx\,dy\;\leqslant\;C_\sigma\;. \quad (F.39)$$

(iv) Finally, for the integral over $(\mathbb{R}^d\setminus B_1)\times B_1$, we have

$$\begin{aligned}&\int_{B_1}\int_{\mathbb{R}^d\setminus B_1}\int_{\mathbb{R}^{d-1}}\frac{|f_{x_d,y}(z')-f_{x_d,y}(x')|}{|x'-z'|^{d-1+2\sigma}}\,dz'dx\,dy \quad (F.40)\\ &\leqslant\;C\int_{|y|\leqslant 1}\int_{|x|>1}\int_{\mathbb{R}^{d-1}}\frac{1}{|x'-z'|^{d-1+2\sigma}}\left|\frac{\phi(y)^2}{|x-y|^{d+1}}-\frac{(\phi(z',x_d)-\phi(y))^2}{|(z',x_d)-y|^{d+1}}\right|dz'dx\,dy\,.\end{aligned}$$

Again, we only need to look at the integral over $|x-y| > 2$ (or any other $r > 0$). In the region where $|x'-z'| > 1$, we have

$$\int_{|y|\leqslant 1}\int_{|x-y|>2}\frac{\phi(y)^2}{|x-y|^{d+1}}\int_{|x'-z'|>1}\frac{1}{|x'-z'|^{d-1+2\sigma}}\,dz'dx\,dy$$
$$\leqslant C\int_2^\infty t^{-2}dt\int_1^\infty s^{-1-2\sigma}ds \;=\; C_\sigma\,,$$

and moreover

$$\int_{|y|\leqslant 1}\int_{|x|>1,|x-y|>2}\int_{|x'-z'|>1}\frac{(\phi(z',x_d)-\phi(y))^2}{|x'-z'|^{d-1+2\sigma}|(z',x_d)-y|^{d+1}}\,dz'dy\,dx$$
$$\leqslant \int_{|y|\leqslant 1}\int_{\mathbb{R}^d}\frac{(\phi(\zeta)-\phi(y))^2}{|\zeta-y|^{d+1}}\int_{|x'-\zeta'|>1}\frac{1}{|x'-\zeta'|^{d-1+2\sigma}}\,dx'd\zeta\,dy$$
$$\leqslant C\int_1^\infty s^{-1-2\sigma}ds\left(\int_0^1 dt+\int_1^\infty t^{-2}dt\right) \;=\; C_\sigma\,,$$

where in the second line we have substituted $\zeta := (z', x_d)$. In the case of $|x'-z'| \leqslant 1$, by the same argument that leads to (F.24), we have for any $\tau \in (0, 1)$ that

$$\left|\frac{\phi(y)^2}{|x-y|^{d+1}}-\frac{(\phi(z',x_d)-\phi(y))^2}{|(z',x_d)-y|^{d+1}}\right| \;\leqslant\; C\,|x'-z'|^\tau\,|x-y|^{-d-\tau}\,,$$

since $|x'-z'| \leqslant |x-y|/2$. Thus, for $\tau \in (2\sigma, 1)$, we have

$$\int_{|y|\leqslant 1}\int_{|x|>1,|x-y|>2}\int_{|x'-z'|\leqslant 1}\frac{1}{|x'-z'|^{d-1+2\sigma}}\left|\frac{\phi(y)^2}{|x-y|^{d+1}}-\frac{(\phi(z',x_d)-\phi(y))^2}{|(z',x_d)-y|^{d+1}}\right|\,dz'dx\,dy$$
$$\leqslant C\int_{|y|\leqslant 1}\int_{|x-y|>2}\frac{1}{|x-y|^{d+\tau}}\,dy\int_0^1 t^{-1+\tau-2\sigma}dt \;=\; C_\sigma\int_2^\infty s^{-1-\tau}\,ds \;=\; C_\sigma\,,$$

and therefore, by (F.40),

$$\int_{B_1}\int_{\mathbb{R}^d\setminus B_1}\int_{\mathbb{R}^{d-1}}\frac{|f_{x_d,y}(z')-f_{x_d,y}(x')|}{|x'-z'|^{d-1+2\sigma}}\,dz'dx\,dy \;\leqslant\; C_\sigma\,. \tag{F.41}$$

Hence, the claim follows from (F.31), (F.35), (F.39), and (F.41). □

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Eidesstattliche Versicherung

Hiermit erkläre ich an Eides statt, dass die vorliegende Dissertation von mir selbständig und ohne unerlaubte Beihilfe angefertigt wurde.

Sebastian Gottwald