Szegő-type asymptotics for the free Dirac operator

Dissertation
an der Fakultät für Mathematik, Informatik und Statistik
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Zusammenfassung

Die Resultate der vorliegenden Dissertation sind maßgeblich durch die Untersuchung von Skalierungsgesetzen der *Verschränkungsentropie* für freie relativistische Fermionen motiviert. Diese stehen im Zusammenhang mit *Szegő-Asymptotiken* für Spektralprojektionen des freien Dirac-Operators, wobei als Testfunktion eine Rényi-Entropiefunktion gewählt wird. Solch eine Spektralprojektion kann als Integraloperator mit einem, möglicherweise unstetigen, matrixwertigen Symbol aufgefasst werden. Im Falle unstetiger skalarwertiger Symbole ist die Szegő-Asymptotik Inhalt der Widom–Sobolev Formel [Sob13]. Eine Anwendung dieser Formel ergibt den Beweis eines *logarithmisch verstärkten Oberflächengesetzes*, also einem führenden Term der Ordnung $L^{d-1} \log L$ bezüglich des Skalierungsparameters L in der Asymptotik, im nicht relativistischen Fall des freien d-dimensionalen Schrödinger-Operators [LSS14]. Die logarithmische Verstärkung tritt auf, falls das Abschneiden an der Fermi-Energie innerhalb des absolutstetigen Spektrums des freien Schrödinger-Operators liegt. Im Fall einer nicht-positiven Fermi-Energie ist das entsprechende Symbol hingegen effektiv glatt und es tritt höchstens ein *Oberflächengesetz*, also ein führender Term der Ordnung L^{d-1}, auf.

Das erste Resultat dieser Dissertation ist in einer Zusammenarbeit mit Peter Müller entstanden [BM24] und ist eine Verallgemeinerung der Widom–Sobolev Formel auf matrixwertige Symbole, welche unstetig auf dem $(d-1)$-dimensionalen Rand eines hinreichend regulären Bereiches sind. Es werden drei, in ihrer Allgemeinheit aufsteigende, Klassen von Testfunktionen betrachtet. Die allgemeinste dieser Klassen enthält die Rényi-Entropiefunktionen. Mit zunehmender Allgemeinheit der Testfunktionen sind striktere Voraussetzungen an die Klasse der zulässigen Symbole verbunden. Auch wenn es für den Anwendungsfall des freien Dirac-Operators nicht nötig ist, werden keine Annahmen an die Kommutativitätseigenschaften des matrixwertigen Symbols benötigt. Der Koeffizient des resultierenden verstärkten Oberflächengesetzes ist genauso explizit wie im skalaren Fall. Dies steht im Gegensatz zur Situation bei glatten Symbolen. Hier ist der Koeffizient des zugehörigen Oberflächengesetzes deutlich weniger explizit für matrixwertige Symbole als für skalarwertige Symbole [Wid80].

Das nächste Resultat, ebenfalls basierend auf der Zusammenarbeit mit Peter Müller [BM25], ist eine Anwendung der bewiesenen Widom–Sobolev Formel für matrixwertige Symbole auf den Spezialfall des freien Dirac-Operators. Da das Spektrum des Dirac-Operators für negative Energien unbeschränkt ist, betrachten wir eine glatt abgeschnittene Version der Fermi-Projektion, um zu garantieren, dass der betrachtete Operator Spurklasse ist. Das Symbol der Projektion erfüllt, abhängig von den beiden Parametern Masse und Fermi-Energie, unterschiedliche Eigenschaften. Wenn, in beliebiger Dimension, der Absolutbetrag der Fermi-Energie strikt größer als die Masse ist oder Fermi-Energie und Masse im eindimensionalen Fall verschwinden, weist das Symbol eine $(d-1)$-dimensionale Unstetigkeit auf und es gilt ein verstärktes Oberflächengesetz. Der dazugehörige Koeffizient ist unabhängig vom glatten Abschneiden der Fermi-Projektion. In den anderen Fällen wird gezeigt, dass höchstens ein Oberflächengesetz auftreten kann.

Ein besonderer Fall tritt auf, falls Fermi-Energie und Masse in einem mindestens zweidimensionalen System verschwinden. In diesem Fall weist das Symbol aufgrund der Struktur des freien Dirac-Operators eine Unstetigkeit in einem einzigen Punkt auf, eine Situation die im nicht relativistischen Fall nicht auftritt. Da diese Unstetigkeit nicht hinreichend für ein verstärktes Oberflächengesetz ist, werden stattdessen die Terme niedrigerer Ordnung der Asymptotik betrachtet. Dazu erfolgt eine Einschränkung auf Würfel als Abschneidebereiche im Ort und analytische Testfunktionen. Das letzte Resultat [Bol25] dieser Dissertation zeigt, dass sich die asymptotische Entwicklung ab dem $(d+1)$ten Term von der Entwicklung für glatte Symbole unterscheidet. Die ersten d Terme der Asymptotik werden bestimmt und es wird bewiesen, dass der übrigbleibende Fehler von logarithmischer Ordnung, $\log L$, ist. Im Spezialfall, dass die Testfunktion ein Polynom von Grad drei oder niedriger ist, wird

eine Entwicklung mit $d + 1$ Termen bewiesen, wobei der zusätzliche Term von logarithmischer Ordnung und der Fehlerterm von konstanter Ordnung ist. Der Koeffizient des logarithmischen Terms ist unabhängig vom glatten Abschneiden der Fermi-Projektion. Die Strategie dieses Beweises beruht auf der Tatsache, dass die inverse Fourier-Transformation des Symbols homogen vom Grad $-d$ ist.

Abstract

The primary motivation behind the results presented in this thesis is the study of scaling laws for the *entanglement entropy* of free relativistic fermions. It is closely related to the *Szegő-type asymptotics* for spectral projections of the free Dirac operator with the test function given by a Rényi entropy function. Such a projection can be written as an integral operator with, potentially discontinuous, matrix-valued symbol. The study of Szegő-type asymptotics for scalar-valued discontinuous symbols is the subject of the Widom–Sobolev formula [Sob13]. As a consequence of this formula, a rigorous proof of a *logarithmically enhanced are law*, i.e. a scaling of leading order $L^{d-1} \log L$ in the scaling parameter L, of the entanglement entropy has been obtained in the non-relativistic case of the free d-dimensional Schrödinger operator [LSS14]. The logarithmic enhancement occurs if the cut-off at the Fermi energy is inside the absolutely continuous spectrum of the free Schrödinger operator. In the case of a non-positive Fermi energy, the symbol of the corresponding pseudo-differential operator is effectively smooth, yielding at most an *area law*, i.e. a scaling of leading order L^{d-1}.

In the first result of this thesis, based on joint work with Peter Müller [BM24], we extend the Widom–Sobolev formula for scalar-valued symbols to matrix-valued symbols which are discontinuous at the $(d-1)$-dimensional boundary of a suitable domain. We consider three different classes of test functions, increasing in generality. The most general of these classes of test functions contains the Rényi entropy functions. As the test functions increase in generality we require more restrictive assumptions on the class of symbols. We do not require any assumptions on the commutation properties of the matrix-valued symbol. The coefficient of the obtained enhanced area term is as explicit as in the scalar-valued case. This is in contrast to the case of a smooth symbol, where the coefficient of the corresponding area law is substantially less explicit in the matrix-valued case [Wid80].

In the next result, also based on joint work with Peter Müller [BM25], we apply the obtained Widom–Sobolev formula for matrix-valued symbols to the special case of the free Dirac operator. Due to the Dirac Sea being unbounded at negative energy levels, we consider a smoothly truncated version of the Fermi projection in order to guarantee that the operator in question is trace class. We analyse the resulting symbol and distinguish between several cases, depending on both mass and Fermi energy. If, in arbitrary dimension, the modulus of the Fermi Energy is strictly larger than the mass, or we have Fermi energy zero in the one-dimensional massless case, the symbol features a suitable $(d-1)$-dimensional discontinuity and we obtain an enhanced area law with coefficient independent of the smooth truncation of the Fermi projection. In the other cases we show that at most an area law holds.

A special case occurs when both Fermi energy and mass vanish in dimension larger than one. In this case, the structure of the free Dirac operator gives rise to a symbol which is discontinuous at a single point, a situation not encountered in the non-relativistic case. As this discontinuity is not sufficient to yield a logarithmic enhancement of the area law, we study the lower-order terms of the asymptotic expansion. We restrict ourselves to analytic test functions and cubes as spatial cut-off domains. We show [Bol25] that the expansion starts to differ from the expansion for smooth symbols starting from the $(d+1)$st term. More explicitly, we obtain the first d terms of the asymptotic expansion and prove that the error obtained by subtracting these first d terms from the expansion is of logarithmic order in the scaling parameter L, instead of being of constant order as in the case of a smooth symbol. In the special case that the test function is a polynomial of degree less or equal than three, we obtain a $(d+1)$-term expansion with the lowest-order term being of order $\log L$ and the error term being of constant order. The coefficient of this logarithmic term is also independent of the smooth truncation of the Fermi projection. The key to the required analysis is the fact that,

in the case of vanishing mass and Fermi energy, the inverse Fourier transform of the symbol is homogeneous of degree $-d$.

Preface

The present thesis consists of two introductory chapters followed by four chapters with a detailed description of the results, including their proofs. The second chapter consists of an introduction to the Widom–Sobolev formula and the free Dirac operator, as well as an overview of the main results of the thesis. The third chapter contains several preparatory estimates which are used in Chapters four and five. The remaining Chapters four to six then contain the main results of the thesis and the corresponding proofs.

Several of the results presented here were obtained in scientific collaboration, which resulted in the publications listed below. The relation to published material is highlighted at the beginning of each of the Chapters two to six. Moreover, parts of the introduction coincide, both in content and writing, with parts of the introductions from the publications (i)-(iii) below.

Published content

(i) L. Bollmann and P. Müller, The Widom–Sobolev formula for discontinuous matrix-valued symbols, *J. Funct. Anal.* **287**, 110651, 54 pp. (2024).

(ii) L. Bollmann and P. Müller, Enhanced area law in the Widom–Sobolev formula for the free Dirac operator in arbitrary dimension, *Pure and Applied Analysis* **7**, 595–613 (2025).

(iii) L. Bollmann, An enhanced term in the Szegő-type asymptotics for the free massless Dirac operator (2025), e-print arXiv:2503.18622, *submitted*.

We do not refer to the publications below by the numbers (i)–(iii) but by their respective abbreviations in the bibliography at the end of this thesis.

Contents

CHAPTER 1

Introduction

First discussed by A. Einstein, B. Podolsky and N. Rosen [EPR35], and taken up shortly after by E. Schrödinger [Sch35, Sch36], *quantum entanglement* is a type of quantum mechanical correlation which is not present in classical mechanics and therefore a distinct feature of quantum mechanics. Since its discovery, entanglement has been extensively studied in large parts of modern physics, ranging from relativity, through quantum optics and statistical mechanics, to quantum information theory and computation [HHHH09, Laf16].

More recently, the *bipartite entanglement entropy* associated to a subregion $\Lambda \subset \mathbb{R}^d$ of d-dimensional Euclidian space has received increased attention. Often the study of *scaling laws* of this entanglement entropy are of key interest [ECP10, Laf16]. These refer to the asymptotic growth of the entanglement entropy with respect to a scaling parameter $L > 0$ as the scaled region $\Lambda_L := \{Lx \in \mathbb{R}^d : x \in \Lambda\}$ grows. This scaling is in general not extensive, i.e. it does not grow with the volume L^d, but the scaling is of lower order. Most typically an area law, i.e. a scaling of order L^{d-1}, or in some cases a (logarithmically) enhanced area law with scaling of order $L^{d-1} \log L$ is observed. The bipartite entanglement entropy has received extensive attention in the study of quantum many-body systems due to its connection to the distribution of quantum correlations in these systems. Intuitively, fast decaying spatial correlations correspond to an area law, as they require interaction to happen close to the boundary of Λ_L. Sometimes this intuition can be made precise as for exponentially decaying correlations in [BH15]. An enhanced area law on the other hand, indicates longer-range correlations, and can therefore serve as as a signature for phenomena like criticality [JK04, RM09, CC09] or delocalisation [MPS20]. If one is able to obtain them, subleading terms of the asymptotic expansion of the entropy are also of great interest, as information about criticality and topological order of the system might only be encoded in these lower-order terms [KP06, FM06, CC09].

The history of area laws for the entanglement entropy dates back to the study of the thermodynamic entropy of black holes. J. Bekenstein argued that this entropy, now referred to as Bekenstein-Hawking entropy, is proportional to the surface area of a black hole [Bek73, Bek04]. Later a relation to the ground state entanglement entropy of free bosonic fields was found, which was first discussed in [BKLS86, Sre93]. Since then area laws have been established for a variety of bosonic and fermionic systems [Laf16]. The relationship between localisation and area laws has also been further investigated, e.g. area laws were established for localised gapped systems with disordered background potential [PS14, EPS17, PS18a]. Especially in two-dimensional systems, there is also interest in the so-called topological term, a subleading term of constant order in the asymptotic expansion which only depends on the topology of Λ [KP06, LW06, HZHL08].

Logarithmically enhanced area laws were first observed in one-dimensional models, e.g. at critical points of XY and XXZ spin chains [VLRK03] and later in conformal field theories [CC09]. In the latter case the enhanced area law is expected to be a purely one-dimensional phenomenon, whereas in dimension two an area law is expected with the criticality of the system being encoded in a subleading term of logarithmic order [FM06, HHCWKM16, CHRE21].

In higher dimensions, the prime example for the occurrence of an enhanced area law is given by the case of the free Fermi gas at zero temperature, where the single-particle Hamiltonian is given by the negative Laplacian. This case has been studied by several authors [Wol06, GK06, HLS11], with a rigorous proof of the enhanced area law given by H. Leschke, A. Sobolev and W. Spitzer [LSS14]. The proof relies on recent progress in the study of *Szegő-type asymptotics* by A. Sobolev [Sob13]. Generalisations of the scaling laws for the free Fermi gas to positive temperatures and towards the inclusion of electric and magnetic background fields were treated, e.g., in [LSS14, LSS17, PS18b, MPS20, MS20, LSS21, Pfe21, LSS22, MS23, PS24a, PS24b]. Another natural way of extending the case of a free Fermi gas is to consider a relativistic system instead of a non-relativistic one, that is to replace the Laplacian, i.e. free Schrödinger operator, by the free Dirac operator as the single-particle Hamiltonian. This is also of interest for non-relativistic systems, as the Dirac equation yields effective descriptions of the low-energy physics of systems as graphene [GN07] or at the surface of three-dimensional topological insulators [HK10]. Understanding the extension to the free Dirac operator is the primary motivation behind the results of the present thesis. The recent paper [FLS24], which is also devoted to a mathematical study of entanglement entropies for a free Fermi gas governed by the Dirac operator, concentrates on the case of Fermi energy $E_F = 0$ and finds a strict area law in dimension $d = 3$, even in the massless case, $m = 0$, where energy zero does not lie in a gap in the spectrum. In the case $d = 1$, with fixed-length intervals instead of scaling domains, a mathematically rigorous result was recently obtained in [FPS24]. The Dirac equation in globally hyperbolic spacetimes with applications to black-hole entropy is discussed in [FL25]. Entanglement signatures of Dirac systems are also a current topic of interest in the physics literature [CWKFF17, ZCHWK18, CHRE21].

The connection between the enhanced area law for the free Fermi gas and the study of Szegő-type asymptotics in the continuum was first observed in [GK06], based on the analysis in [Kli06]. In the present thesis we also take the route of studying Szegő-type asymptotics, now for matrix-valued symbols, in order to gain insights on (logarithmically) enhanced terms occurring in the asymptotic entropy expansion of the free Dirac operator. This both explains the title of the present thesis and motivates the following overview on developments in the field of Szegő-type asymptotics. The study of Szegő-type asymptotics dates back to the analysis of the determinant of large Toeplitz matrices initiated by Szegő [Sze15]. Let $a : \mathbb{T} \to \mathbb{R}$ be a strictly positive function on the torus $\mathbb{T}$ with Fourier coefficients $(a_j)_{j\in\mathbb{Z}}$. Consider the (infinite) Toeplitz matrix $T := (a_{j-k})_{j,k\in\mathbb{N}}$ and, for a scaling parameter $L \in \mathbb{N}$, its finite-volume truncation $T_L := (a_{j-k})_{1\leqslant j,k\leqslant L}$. Under these assumptions Szegő [Sze15] obtained the asymptotic expansion

$$\log\det(T_L) = L(\log a)_0 + o(L), \tag{1.1}$$

as $L \to \infty$. Here $(f)_k$ denotes the kth Fourier coefficient of the function f. In [Sze20] he extended (1.1) from the natural logarithm log to Riemann integrable test functions h:

$$\operatorname{tr} h(T_L) = L(h \circ a)_0 + o(L), \qquad \text{as } L \to \infty. \tag{1.2}$$

The next big step [Sze52] was to find the subleading term of this asymptotic expansion which, for sufficiently smooth positive symbols a, turned out to be of constant order, leading to an expansion of the form

$$\log\det(T_L) = L(\log a)_0 + \sum_{l=1}^{\infty} l(\log a)_l(\log a)_{-l} + o(1), \qquad \text{as } L \to \infty. \tag{1.3}$$

In further publications the assumption on the symbol a were weakened, see e.g. [Bax63, Hir66]. The question of the nature of the coefficient of the constant order in (1.3) for more general test functions, was answered by L. Libkind [Lib72] with the formula

$$\operatorname{tr}(h(T_L)) = L(h \circ a)_0 + W_1(h; a) + o(1), \qquad \text{as } L \to \infty, \tag{1.4}$$

for analytic test functions h and with coefficient

$$W_1(h;a) = \frac{1}{4\pi^2}\sum_{k=1}^{\infty}\int_{\mathbb{T}}\int_{\mathbb{T}}\frac{a(x)h(a(y)) - a(y)h(a(x))}{a(x)-a(y)}\Big(\frac{a'(x)}{a(x)} - \frac{a'(y)}{a(y)}\Big)\sin k(x-y)\,\mathrm{d}x\,\mathrm{d}y. \quad (1.5)$$

A two-term expansion as in (1.3) has also been obtained in the case that the symbol a is no longer real-valued but instead matrix-valued [Wid75].

The order of the second term in (1.3) respectively (1.4) crucially depends on the continuity of the symbol a. For symbols with jump discontinuities the second term features a logarithmic enhancement [FH69, Wid73, Wid76, Bas86], i.e. the obtained expansion is of the form

$$\operatorname{tr}(h(T_L)) = L(\log a)_0 + \log L\; W(h;a) + o(\log L), \qquad \text{as } L \to \infty, \quad (1.6)$$

with a coefficient $W(h;a)$ depending on the test function h and the values of the symbol a at its jump discontinuities. In the present thesis we are mainly interested in continuous analogues of these discrete Szegő-type asymptotic expansion, where the Toeplitz matrices are replaced by Wiener–Hopf operators. We refer to [BS99, BS06, DIK11] for further discussion on the Toeplitz matrix case.

In the continuum case the role of the symbol is played by a sufficiently smooth complex-valued function $a : \mathbb{R}^d \to \mathbb{C}$. As in the discrete case two distinct situations, depending on the smoothness of the symbol, are studied. In the case of a symbol without discontinuities, the Wiener–Hopf operator with action

$$(T_L u)(x) = \frac{1}{(2\pi)^d}1_{\Lambda_L}(x)\int_{\mathbb{R}^d}\int_{\Lambda_L} \mathrm{e}^{\mathrm{i}\xi(x-y)}\, a(\xi)u(y)\,\mathrm{d}y\,\mathrm{d}\xi, \qquad x \in \mathbb{R}^d, \quad (1.7)$$

on Schwartz functions $u \in \mathcal{S}(\mathbb{R}^d)$ is considered. Here, Λ_L is a sufficiently regular bounded domain scaled with the scaling parameter $L > 0$. While the operator in (1.7) could also be written in terms of the the Fourier transform $\mathcal{F}$ on $L^2(\mathbb{R}^d)$, we chose to write it as a double integral operator here, as beginning with Chapter 2 we also consider symbols $a : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$ which depend on both position and momentum space, making the notation in (1.7) more suitable. For this operator, a two-term asymptotic formula with a leading volume term and a subsequent surface area term, i.e. of the form

$$\operatorname{tr}_{L^2(\mathbb{R}^d)}[h(T_L)] = L^d W_0(h;a) + L^{d-1}W_1(h;a) + o(L^{d-1}), \quad (1.8)$$

is established for analytic or smooth test functions. For one-dimensional scalar-valued symbols this was proved in [Kac54], for higher-dimensional scalar-valued symbols this was proved, each time under different assumptions, in [Wid60, Lin75, Wid74]. An extension to matrix-valued symbols, generalising the one-dimensional Toeplitz matrix analogue, is contained in [Wid80]. Here, the coefficient of the (surface) area term is given by

$$W_1(h;a) := \frac{1}{(2\pi)^{d-1}}\int_{T^*\partial\Lambda} \operatorname{tr}_{L^2(\mathbb{R}_+)\otimes\mathbb{C}^n}[h(W(a_X)) - W(h(a_X))]\,\mathrm{d}X, \quad (1.9)$$

where $X = (x,\eta)$ is a point in the (suitable identification of the) cotangent bundle $T^*\partial\Lambda$ of $\partial\Lambda$ with $x \in \partial\Lambda$ and η orthogonal to the unit normal vector ν_x of $\partial\Lambda$, $\mathrm{d}X$ is the canonical volume element of $T^*\partial\Lambda$ and $W : L^2(\mathbb{R}_+)\otimes\mathbb{C}^n \times L^2(\mathbb{R}_+)\otimes\mathbb{C}^n$ is the one-dimensional Wiener–Hopf operator with symbol $a_X : \mathbb{R} \ni \xi \mapsto a(\eta + \xi\nu_x) \in \mathbb{C}^{n\times n}$. Due to the absence of an analogue to the formula by L. Libkind, a simpler expression for the trace in the integrand, akin to (1.5), is in general not known. This makes the coefficient substantially less explicit than in the scalar-valued case, as the trace of the one-dimensional Wiener–Hopf operator remains.

With the increased interest in scaling laws for the entanglement entropy, more general test functions were considered which include the von-Neumann and Rényi entropy functions. The expansion (1.8) was extended to these test functions for scalar-valued symbols in [Sob19] and matrix-valued symbols in [FLS24].

For analytic, and in some cases sufficiently smooth, test functions, it is also possible to obtain additional terms in the asymptotic expansion. For domains with C^3-boundary a three-term asymptotic expansion was obtained in [Roc84]. In [Wid85], for arbitrary $m \in \mathbb{N}$ and domains with C^∞-boundary, an asymptotic expansion

$$\operatorname{tr}_{L^2(\mathbb{R}^d)}[h(T_L)] = \sum_{k=0}^{m} L^{d-k} W_k(h;a) + o(L^{d-m}), \qquad \text{as } L \to \infty, \tag{1.10}$$

with recursively defined coefficients $W_k(h;a)$ was obtained. More recently, domains with only piece-wise smooth boundary have been considered. In [Die18] a complete $(d+1)$-term expansion of the form

$$\operatorname{tr}_{L^2(\mathbb{R}^d)}[h(T_L)] = \sum_{k=0}^{d} L^{d-k} W_k(h;a) + o(L^{-\tau}), \qquad \text{as } L \to \infty, \tag{1.11}$$

was established in the case that Λ is a d-dimensional cube, where $\tau > 0$ depends on the rate of decay of the operator kernel of T_L. This result holds in the more general setting of $\mathbb{Z}^d$-ergodic operators. The article [Pfi19] considers two-dimensional polygons and proves a complete three-term expansion of the form (1.11) for smooth, i.e. C^∞, symbols and with $\tau > 0$ arbitrarily large. An expansion similar to (1.11) was also established for analytic test functions in the discrete, i.e. Toeplitz matrix, case in [Tho96].

The case of a discontinuous symbol, traditionally refers to the symbol having a $(d-1)$-dimensional discontinuity in momentum space at the boundary of a sufficiently regular bounded domain $\Gamma \subset \mathbb{R}^d$. Then the action of the Wiener–Hopf operator on $u \in \mathcal{S}(\mathbb{R}^d)$ reads

$$(T_L u)(x) = \frac{1}{(2\pi)^d} 1_{\Lambda_L}(x) \int_\Gamma \int_{\Lambda_L} \mathrm{e}^{\mathrm{i}\xi(x-y)}\, a(\xi) u(y)\, \mathrm{d}y\, \mathrm{d}\xi, \qquad x \in \mathbb{R}^d, \tag{1.12}$$

compared to (1.7). In this case one obtains a two-term asymptotic with a leading volume term and a subsequent logarithmically enhanced area term, i.e. of the form

$$\operatorname{tr}_{L^2(\mathbb{R}^d)}[h(T_L)] = L^d W_0(h;a) + L^{d-1} \log L\; W_1(h;a) + o(L^{d-1}\log L). \tag{1.13}$$

The coefficient $W_1(h;a)$ of the enhanced area law depends on both the discontinuities at $\partial\Lambda$ and $\partial\Gamma$. In dimensions $d \geqslant 2$, it is given as an explicit double integral over the boundaries $\partial\Lambda$ and $\partial\Gamma$, see (2.16). The progress of proving the expansion (1.13) has been considerably slower than in the case without discontinuity. In one spatial dimension (1.13) was proved in [LW80] and [Wid82], where in the latter case the error term is of constant order, due to a different technique of proof. Also in [Wid82] the expansion (1.13) together with the concrete expression of the coefficient $W_1(h;a)$ was conjectured for the first time. The first step in proving the higher-dimensional case, then known as Widom's conjecture, was a proof of the special case where Γ is a half-space in [Wid90]. Here, the error term is of order L^{d-1}. It took over two additional decades until the proof of Widom's conjecture, now known as the Widom–Sobolev formula, by A. Sobolev in [Sob13] with an extension to only piece-wise regular domains in [Sob15]. In this general case, the error term is as in (1.13) and, in contrast to the case of a continuous symbol, the lower-order terms are not known. The enhanced area law for the free Fermi gas is a consequence of the Widom–Sobolev formula. The extension from smooth test functions to the non-smooth Rényi entropy functions for certain symbols a in [LSS14] was achieved using the Schatten–von Neumann class bounds in [Sob14]. An extension of the general two-term Widom–Sobolev formula to a more general class of test functions, containing all Rényi entropy functions, was obtained in [Sob17].

While the one-dimensional formula in [Wid82] was also stated for matrix-valued symbols, the higher dimensional Widom–Sobolev formula for matrix valued symbols was proved in [BM24] and constitutes one of the parts of the present thesis. Here, the coefficient W_1 is as explicit as in the scalar-valued case, in contrast to the coefficient W_1 in the case with continuous symbol, cf. (1.9) and (1.5). The systematic route towards an enhanced area law for matrix-valued symbols in higher dimensions consists of generalising appropriate parts of the scalar-valued results [Sob13, Sob14, Sob15, Sob17] to matrix-valued symbols. This is the content of the first result contained in this thesis.

In this first part we prove several variants of the Widom–Sobolev formula for traces of test functions of truncated Wiener–Hopf operators with matrix-valued symbols. The three main results are expansions for analytic test functions h, for arbitrarily often differentiable h and for test functions h which are twice differentiable except at finitely many points where they merely obey a Hölder condition, see Assumption 2.5. Notably, the last class of test functions includes all Rényi entropy functions, in particular the von Neumann entropy function. The study of the entanglement entropy is the primary motivation to consider this last class of test functions. In contrast to the test functions, the allowed Wiener–Hopf operators decrease in generality from analytic test functions to the more general test functions. For example, the truncated Wiener–Hopf operator for arbitrarily often differentiable test functions is of the form

$$\begin{aligned} G_L(A_1, A_2; \Lambda, \Gamma) := {} & \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Re}\big[\operatorname{Op}_L^l(\operatorname{Re} A_1)\big] \operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda \\ & + \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \operatorname{Re}\big[\operatorname{Op}_L^l(\operatorname{Re} A_2)\big] \operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Lambda, \end{aligned} \tag{1.14}$$

where A_1 and A_2 are suitable smooth symbols with values in the $\mathbb{C}^{n\times n}$-matrices which may depend on both position and momentum. The (standard) left-quantisation functor Op_L^l of the symbols is defined in (2.20), and $\operatorname{Re} T := (T + T^*)/2$ is the self-adjoint part of a (bounded) operator T. Besides the discontinuity in position space due to the restriction to the volume $\Lambda \subset \mathbb{R}^d$, the truncated Wiener–Hopf operator (1.14) features a second, more general jump discontinuity at the boundary of the momentum region $\Gamma \subset \mathbb{R}^d$ where the change from A_1 to A_2 occurs. Because of the two discontinuities, we obtain the two-term asymptotic expansion

$$\begin{aligned} &\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(G_L(A_1, A_2; \Lambda, \Gamma)\big)\big] \\ &\qquad = L^d\Big[\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(\operatorname{Re} A_1)]; \Lambda, \Gamma\big) + \mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(\operatorname{Re} A_2)]; \Lambda, \Gamma^c\big)\Big] \\ &\qquad\quad + L^{d-1}\log L\, \mathfrak{W}_1\big(\mathfrak{U}(h; \operatorname{Re} A_1, \operatorname{Re} A_2); \partial\Lambda, \partial\Gamma\big) \\ &\qquad\quad + o(L^{d-1}\log L), \end{aligned} \tag{1.15}$$

as $L \to \infty$ with a logarithmically enhanced area term. Interestingly, the coefficients $\mathfrak{W}_0$ and $\mathfrak{W}_1$ are the same as in the scalar case, see (2.15) and (2.16). For $d = 1$, this was already found by H. Widom [Wid82]. We point out that the first argument of $\mathfrak{W}_0$ is a matrix trace and, hence, scalar valued. The same is true for the first argument of $\mathfrak{W}_1$, where the matrix trace is hidden in the definition (2.32) of the scalar-valued symbol $\mathfrak{U}$, cf. (2.32).

An operator sum as in (1.14) describes the general jump discontinuity of a symbol along the boundary of Γ. This type of discontinuity will be crucial when we turn to the application to the free Dirac operator in the next result. However, it also represents an additional technical challenge if the matrix-valued symbols A_1 and A_2 do not commute. A careful consideration in the proof of Theorem 4.5 still allows us to obtain coefficients similar to the scalar-valued case. Such operator sums were first studied in [Sob17, Thm. 5.2] for scalar-valued symbols. In addition to working with matrix-valued symbols, we require slightly weaker assumptions on Γ and on the symbols A_1 and A_2. The first situation requires either Γ or Γ^c to be bounded. Then, only one symbol needs to have compact support in momentum, namely the one that is in the same term of (1.14) as the unbounded momentum region. The second situation allows both Γ and Γ^c to be unbounded. But then, both symbols A_1 and A_2 are required to be compactly supported in momentum. These less stringent requirements stem from less stringent requirements in some Schatten–von Neumann estimates that we prove in Chapter 3. This fact also simplifies several steps leading to the desired variants of the Widom–Sobolev formula.

The extension of (1.15) from polynomial test functions h to more general test functions is often referred to as the "closing of the asymptotics". Given a single scalar-valued symbol A_1, i.e. $A_2 = 0$, the results for different classes of test functions and (merely piece-wise) differentiable admissible domains Λ and Γ can be assembled from different papers within the large body of work of A. Sobolev [Sob13, Sob14, Sob15, Sob17] with precursors by H. Widom [Wid90] and D. Gioev [Gio06]. In this thesis, we give a unified and complete treatment of such results for matrix-valued symbols, without sacrificing too much generality for a given class of test functions.

With the Widom–Sobolev formula for matrix-valued symbols and the entropy functions at hand, our the next step is to apply it to the special case of the free Dirac operator. Our main focus here is on situations which lead to a logarithmically enhanced area law of the entanglement entropy. The goal is to obtain these enhanced area laws from the Widom–Sobolev formula in a similar fashion as in the the corresponding non-relativistic case for the Laplacian [LSS14]. But in contrast to this non-relativistic case, one has to cope with several additional difficulties in order to achieve this. This can be seen by taking a closer look at the symbol $1_{E_F}(D)$ of the operator obtained through application of the Fermi projection 1_{E_F}, at a given Fermi energy $E_F \in \mathbb{R}$, to the free Dirac operator. We first note that this symbol is not integrable, as the spectrum of the free Dirac operator is given by $]-\infty, m] \cup [m, \infty[$, with mass $m \geqslant 0$, and is therefore not bounded from below. Hence, the operator $T_L(1_{E_F}(D))$ is not trace class. To remedy this problem we introduce a suitable smooth cut-off of the Dirac sea at negative energies. In order for this to be a meaningful procedure, we then prove that the leading-order coefficient of the asymptotic expansion is independent of the choice of smooth cut-off function.

The presence of two spectral bands at positive and negative energies also leads to complications in the geometric structure of the relevant regions in momentum space. For this reason we distinguish between several different cases in the application, depending on the relevant regions in momentum space. Whereas for the Laplacian [LSS14] the relevant region in momentum space is the interior of the bounded Fermi ball, the relevant momenta for the Dirac operator also lie in the unbounded complement of a ball. The smooth cut-off of the Fermi projection then guarantees that the symbol is still compactly supported in this unbounded complement. We note here that the fact, that both the unbounded region and the support of the symbol are in momentum space, leads to a different situation from the one where an unbounded spatial region Λ with bounded complement is studied, e.g. in [LSS16, LSS17, Sob19, FLS24]. While in the latter case it suffices to subtract an operator corresponding to an infinite volume term in order to obtain a trace-class operator, cf. the proof of Corollary 4.7, in our case this is not sufficient, as also the subleading terms are not well-defined without a smooth cut-off, cf. [FLS24]. Moreover, in the Laplacian case the symbol always vanishes on one side of the discontinuity in momentum space. Here, we need to cope with symbols that take on non-zero values on both sides of the discontinuity. But this is exactly the structure of the operator in (1.14) which makes the expansion (1.15) particularly suited for this application.

Overcoming these difficulties [BM25], we obtain logarithmically enhanced area laws for the trace of rather general functions – including all Rényi entropy functions – in the cases $|E_F| > m$ in all space dimensions $d \in \mathbb{N}$ and $E_F = m = 0$ in $d = 1$, where the discontinuity of the symbol $1_{E_F}(D)$ at the Fermi surface is a $(d-1)$-dimensional object. In the complementary cases, i.e. $|E_F| \leqslant m \neq 0$ for any d and $E_F = m = 0$ in $d \geqslant 2$, the coefficient of the enhanced area law vanishes, and we perform some further analysis to show that the corrections grow at most of the order of the area. While such a behaviour is not at all surprising in the spectral-gap case $|E_F| \leqslant m \neq 0$, where the Fermi-surface vanishes, the interesting case $E_F = m = 0$ in $d \geqslant 2$ still features a zero-dimensional discontinuity of the symbol $1_{E_F}(D)$ at the origin. Still, we show that this zero-dimensional discontinuity is not sufficient to induce a logarithmic enhancement of the area law in dimensions $d \geqslant 2$, as it is too low dimensional. From what has been said above, the point discontinuity of the symbol at the origin is sufficient, however, to induce a logarithmic enhancement in $d = 1$.

It is expected that the case $E_F = m = 0$ plays a special role, as it corresponds to the quantum critical Dirac point where the two Dirac cones, of the dispersion relation corresponding to the massless Dirac equation, meet. But, as our second result shows, this criticality does not lead to an enhanced area law for the entanglement entropy in higher dimensions. Therefore, the natural question arises whether and to which extent this criticality plays a role in the asymptotic expansion of the entropy. Is this somehow encoded in a lower-order term of the expansion or is the expansion unaffected and as in the gapped case? And if there is a lower-order term, does it depend on the smooth cut-off of the Fermi projection or is it independent of the chosen cut-off? These questions directly correspond to questions about Szegő-type asymptotics in the continuum. What happens if, instead of a symbol with no discontinuity or one with a $(d-1)$-dimensional discontinuity, we consider a symbol with a zero-dimensional discontinuity? Is the expansion as the one for continuous symbols, or does one find an enhanced term of lower order? And if one obtains such a lower-order term, does its coefficient only depend on the value the symbol takes on at the point of discontinuity, as in the case of the enhanced area law in the Widom–Sobolev formula? Can one even find an explicit integral representation of such a coefficient somehow relating it to the one in the Widom–Sobolev formula?

To, at least partially, answer these questions is the goal of the last result of the present thesis [Bol25]. As the leading and next to leading order terms are of the same order as the corresponding terms for continuous symbols, the aim is to study the terms of even lower order until the effect of the discontinuity on the asymptotic expansion becomes apparent. As the study of the lower-order terms is in general quite challenging, we not only make use of the zero-dimensional discontinuity but also of some parts of the concrete structure of the free Dirac operator. This allows to also consider the symbol from the following point of view: The inverse Fourier transform of the symbol $1_{E_F}(D)$, i.e. the integral kernel of the studied operator can be written as a sum of d-dimensional Riesz transforms. These are homogeneous of degree $-d$, leading to an off-diagonal decay of order $|x - y|^{-d}$ for the integral kernel.

Comparing this decay with the decay faster than of order $|x - y|^{-(d+1)/2}$, required to obtain the area term for continuous symbols and quadratic test functions, e.g. in [Wid80], allows us to develop an intuition about the structure of the expansion. The difference of just less than $(d-1)/2$ in the order, combined with the fact that $L^2(\mathbb{R}^d \times \mathbb{R}^d)$-bounds of the kernel correspond to Hilbert-Schmidt bounds of the operator, suggests that one might be able to prove that an additional number of $d-2$ terms (for a total number of d terms) of the asymptotic expansion are of the same order as in the case with continuous symbol. Therefore, the structure of the expansions could only begin to differ starting from the $(d+1)$st term. Similarly, the zero-dimensional discontinuity also allows us to gain some intuitive insights. As in the one-dimensional case $E_F = m = 0$ in our second result, one might expect a logarithmically enhanced term of order $\log L$. Furthermore, in analogy to the interaction of the two $(d-1)$-dimensional boundaries $\partial\Lambda$ and $\partial\Gamma$ in the enhanced area coefficient of the Widom–Sobolev formula, one might suspect an interaction of the zero-dimensional discontinuity with zero-dimensional points in the boundary of Λ, where the smoothness of the boundary breaks down, e.g. the vertices of a d-dimensional cube. The occurrence of a lower-order logarithmic term and its dependence on the corners of the spatial restriction are also discussed in the physics literature, see e.g. [FM06, CH09, CHL09, KSFSM14, HHCWKM16, HLHM19, CHRE21].

Due to the aforementioned interest in the interaction with vertices, we are especially interested in studying domains Λ with only piece-wise smooth boundary. We have chosen to restrict ourselves to d-dimensional cubes, as they still have a sufficiently simple structure in higher dimensions, which helps us illustrate the general structure of the asymptotic expansion depending on the dimension d. Furthermore, we can use the already established $(d+1)$-term expansions for cubes in the case of continuous symbols [Die18] as a starting point. We also restrict ourselves to analytic test functions h with $h(0) = 0$ as in most of the already obtained higher-order asymptotic expansions for continuous symbols. Although it would certainly be desirable to also be able to treat the entropy functions, the strategy to deal with these more general functions, laid out in [Sob17], is based on utilising the quasi-commutator structure of the relevant operators which is incompatible with the reduction strategy we use to obtain the higher-order asymptotic expansion. We are unaware of any way to remedy this problem. With these restrictions we expect an asymptotic expansion of the following form

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}[h(T_L(D_b))] = \sum_{k=0}^{d-1} L^{d-k} W_k(h; D_b) + \log L\, W(h; D) + o(\log L), \qquad \text{as } L \to \infty, \tag{1.16}$$

to hold. Here, the operator $T_L(D_b)$ depends on the matrix-valued symbol $D_b : \mathbb{R}^d \to \mathbb{C}^{n\times n}$ which stems from the regularised Fermi projection of the Dirac operator and depends on the parameter $b \geqslant 0$ determining the regularisation. We note that the coefficient of the logarithmic term $W(h; D)$ is independent of the cut-off parameter b. Unfortunately, we are only able to prove the whole expansion (1.16) for polynomial test functions of sufficiently low degree, for reasons explained in the next paragraph and in Chapter 6. For general analytic test functions we still manage to obtain the first d terms of the expansion and prove an upper bound, logarithmic in L and independent of the cut-off parameter b, for the remaining term.

In order to prove the desired asymptotic expansion (1.16), we combine techniques from both the analysis of continuous and discontinuous symbols. We obtain the first d terms of the expansion in a similar way as for smooth symbols. While the algebraic decomposition of the cube works in a similar way as in [Die18], the substantially worse decay of the kernel forces us to obtain the required estimates in a different way. We instead obtain Hilbert-Schmidt estimates from the integral kernel decay, where we use a quite technical procedure of constructing neighbourhoods of certain regions in position space whose boundaries locally are graphs of suitably chosen power functions $f(x) = x^q$ with $0 < q < 1$. This procedure is best illustrated in the proof of Lemma 6.11. After finding the first d terms of the expansion, we treat the remaining operator in a similar way as in the case of a discontinuous symbol, cf., e.g., [Wid82, Sob15]. We first prepare the operator by reducing it to a sum of vertex contributions through localisation and commute out the smooth regularisations of the Fermi projection. As we are only allowed to incur error terms of constant order while doing so, we need to make use of the structure of the remaining operator. After this preparation, we further follow the strategy for discontinuous symbols and provide a local asymptotic formula. The integral kernel of the prepared operator is a generalisation of the kernel in the one-dimensional case, where the occurring Hilbert transform is replaced by its higher dimensional analogues, the Riesz transforms. Therefore, the idea is to extend the original one-dimensional proof in [Wid82] to higher dimensions. While doing so, we face the challenge that the one-dimensional proof relies on a connection between Hilbert and Mellin transform which allows one to find the spectral representation of the Wiener–Hopf operator in question. This is the point were we need to restrict our choice of test functions, as we are not able to find a higher-dimensional analogue to this connection. This is due to the substantially more complex structure of the higher-dimensional operator and the unclear connection between the higher-dimensional transforms. Still, we are able to prove the required properties of the kernel by hand and a local asymptotic formula in the special case that the test function is given by a polynomial of degree three or less. For general analytic test functions, we instead obtain a logarithmic upper bound for the remaining operator in a similar way as the upper bounds in our second result [BM25].

Structure of the thesis: The thesis is organised as follows: In Chapter 2 we give a mathematical introduction to the Widom–Sobolev formula, pseudo-differential operators with matrix-valued symbols and the free Dirac operator in the context of the present thesis. Moreover, we give an overview of the main results of the thesis. In Chapter 3 we prove several bounds for pseudo-differential operators with matrix-valued symbols which will be needed in Chapters 4 and 5. In Chapters 4 - 6 we then present the main results from the introduction in detail and give the corresponding proofs. All of these chapters are organised in a similar manner. We begin by discussing the results as well as the required assumptions and, if applicable, also related open questions. Due to the aspiration that these chapters can be read independently of the introduction, these parts necessarily contain some overlap with both introductory chapters. Next, we discuss the strategy and key ideas of the corresponding proofs, often in a simplified case. Finally, we prove the respective results in full detail.

Some remarks on notation: We try to follow standard notational conventions and describe the relevant notation upon its first introduction. Large parts of the relevant notation are introduced in Chapter 2. Chapters 4 - 6 are intended to be readable largely independently of one another, although Chapter 4 and to some degree Chapter 5 require the results of Chapter 3. We also recall some of the relevant notation at the beginning of the respective chapters and their sections. We try to maintain a coherent notation throughout the entirety of the thesis. Excluded from this, is the use of constants which is different in Chapters 3 and 4. Usually, we number constants along the lines of $C_1, C_2, \dots$ or $C', C'', \dots$ in a single given proof. After the conclusion of the proof, the numbering resets. In Chapters 3 and 4 however, we use the letters $C, C_1, C_2, C_{\nu\mu}$, etc. to denote generic positive constants whose value may differ from line to line, as otherwise the readability of the corresponding proofs would suffer. We recall this fact at the beginning of the respective chapters.

CHAPTER 2

Mathematical background and main results

Context: This chapter contains an introduction to the objects studied in the Widom–Sobolev formula and to the free Dirac operator. We focus on the material most important to the present thesis. After the necessary preliminaries are established, the main results of the thesis are stated in a slightly simplified form. Both content and writing in this chapter largely agree with the respective content of the introductory sections of [BM24] and [BM25], both collaborations with Peter Müller, as well as [Bol25].

Content: In the first section we give an overview of the Widom–Sobolev formula in both the scalar- and matrix-valued case. We introduce the required objects with a focus on pseudo-differential operators with matrix-valued symbols and give an overview of the main results contained in Chapter 4. We only give a treatment of pseudo-differential operators to the extent it is required for the Widom–Sobolev formula. For a more general overview on pseudo-differential operators with semi-classical parameter we refer to [DS99] and for the classical case to [Hör07].

The second section gives an introduction to the free Dirac operator. We investigate the application of bounded, measurable functions to the operator and interpret the result in the context of the more general pseudo-differential operators with matrix-valued symbols, established in the first section. We only focus on the aspects most relevant to the present thesis. For a more general overview on the Dirac equation, we refer to, e.g., [BS57, Tha92]. We also discuss the relation of the Widom–Sobolev formula and scaling laws of entanglement entropy, as well as state the main result of Chapter 5.

In the third section we take a closer look at the special case of the massless Dirac operator. We discuss the properties of the arising matrix-valued symbol and give an overview of the main results contained in Chapter 6.

2.1. The Widom–Sobolev formula

The Widom–Sobolev formula is based on a famous conjecture by H. Widom [Wid82], where it was also proven in the one-dimensional case. The higher dimensional cases were famously proven by A.V. Sobolev in [Sob13] and extended in [Sob14, Sob15, Sob17]. The formula gives a two-term asymptotic expansion, in the scaling parameter $L > 0$, for the trace of the following operator

$$h\big(1_\Lambda \operatorname{Op}_L(1_\Gamma) \operatorname{Op}_L^l(a) \operatorname{Op}_L(1_\Gamma) 1_\Lambda\big). \tag{2.1}$$

Here, a is called a symbol, 1_Λ and 1_Γ are projections on some sufficiently regular domains $\Lambda, \Gamma \subseteq \mathbb{R}^d$, Op_L^l denotes the left (pseudo-differential) operator with semi-classical scaling parameter L and h is called a test function. In this section we provide details on each of the objects contained in the operator (2.1), as well as define the coefficients arising in the corresponding asymptotic formula.

2.1.1. Admissible domains. We begin by defining the types of domains studied in this thesis and which are suitable for the Widom–Sobolev formula. Here, we mostly follow the terminology in [Sob14].

Definition 2.1. Given a natural number $d \in \mathbb{N} \setminus \{1\}$, we call a subset $\Omega \subset \mathbb{R}^d$ a *basic domain*, if there exists a Lipschitz function $\Phi : \mathbb{R}^{d-1} \longrightarrow \mathbb{R}$ and a suitable choice (obtained by relabelling and rotation) of Cartesian coordinates $\mathbb{R}^d \ni x = (x_1, x_2, \ldots, x_d)$ such that

$$\Omega = \big\{x \in \mathbb{R}^d : x_d > \Phi(x_1, x_2, \ldots, x_{d-1})\big\}. \tag{2.2}$$

For $m \in \mathbb{N} \setminus \{1\}$, we further call a basic domain a *piece-wise C^m-basic domain*, if, in addition, Φ is a piece-wise C^m-function. In the case $d = 1$, we call $\Omega \subset \mathbb{R}$ a (piece-wise C^m-) basic domain, if it is an open interval of the form $]a, \infty[$, respectively $]-\infty, a[$, for arbitrary $a \in \mathbb{R}$.

Definition 2.2. We call $\Omega \subseteq \mathbb{R}^d$ an *admissible domain*, if it can be locally represented as a basic domain, i.e. for all $x \in \mathbb{R}^d$ there is some $r_x > 0$ such that for $B_{r_x}(x)$, the open ball of radius r_x about x in $\mathbb{R}^d$, we have

$$B_{r_x}(x) \cap \Omega = B_{r_x}(x) \cap \Omega_x \tag{2.3}$$

for some basic domain Ω_x. For $m \in \mathbb{N}$, we further call an admissible domain a *piece-wise C^m-admissible domain*, if it can be locally represented as a piece-wise C^m-basic domain, i.e. the domains Ω_x in (2.3) are piece-wise C^m-basic domains.

Remark 2.3. (a) Given a basic domain Ω_0, the domain $\big(\overline{\Omega_0}\big)^c$ is also a basic domain by the coordinate transformation $x_d \mapsto -x_d$ and replacing Φ by $-\Phi$. This extends to admissible domains in the following way. Given an admissible domain Ω, locally represented by basic domains Ω_x, the domain $\big(\overline{\Omega}\big)^c$ is locally represented by the basic domains $\big(\overline{\Omega_x}\big)^c$ and therefore again admissible.
(b) We note that the boundary of a basic domain has Lebesgue measure zero as it is the graph of a Lipschitz function. This also extends to admissible domains, as $\mathbb{R}^d$ is heredetarily Lindelöf – every metrisable space is heredetarily Lindelöf, see, e.g., [Eng89, Ex. 3.8.A, Cor. 4.1.13] – and therefore each open cover of the boundary has a countable subcover.
(c) Given an admissible domain Ω, the operator 1_{Ω^c} of multiplication with the indicator function of Ω^c agrees with the operator $1_{(\overline{\Omega})^c}$ on $L^2(\mathbb{R}^d)$, as $\partial\Omega$ has (Lebesgue) measure zero. Therefore, the operator 1_{Ω^c} acts as multiplication with the indicator function of an admissible domain. This will be utilised quite often in the later chapters of this thesis.

We now give a simple example of an admissible domain which, nevertheless, plays a major role in Chapter 6 of the present thesis.

Example 2.4. Let $\Omega :=]-a, a[^{\,d} + b \subset \mathbb{R}^d$ be a d-dimensional cube of side-length $2a > 0$ centred about $b \in \mathbb{R}^d$. Then Ω is a piece-wise C^∞-admissible domain. While elementary, it still is useful to give a sketch of the argument, in order to become more accustomed to the analysis of the cube featured in Chapter 6:

In the cases where x is not in the boundary $\partial\Omega$ of Ω, we find some radius $r_x > 0$ such that the cube Ω agrees with either $\mathbb{R}^d$ or $\emptyset$ in the ball $B_{r_x}(x)$ and the corresponding C^∞-basic domains are easily obtained. As usual, for $k \in \{0, \ldots, d\}$, we call $F \subseteq \mathbb{R}^d$ a k-face (of Ω) if the dimension of the smallest affine subspace of $\mathbb{R}^d$ containing F is equal to k (we write this as $\dim(F) = k$) and there exists a half-space $H_F \subseteq \mathbb{R}^d$ with $\Omega^\circ \cap \partial H_F = \emptyset$ such that $F = \overline{\Omega} \cap H_F$. If now $x \in \partial\Omega$, there exists a minimal dimension $m \in \{1, \ldots, d-1\}$, such that x is contained in a face of dimension m. This face is unique, as otherwise the intersection of the two faces would be a face of dimension lower than m which still contains x. In the case $m = d - 1$, we see that, after suitable rotation and translation, the cube Ω is locally represented by the basic domain Ω_x with (piece-wise) C^∞-function Φ_x given by $\Phi_x(x_1, x_2, \ldots, x_{d-1}) := 0$. In the case $m = d - 2$, the piece-wise C^∞-function Φ_x is, after suitable rotation and translation, instead given by $\Phi_x(x_1, x_2, \ldots, x_{d-1}) := |x_1|$. For $m \in \{0, \ldots, d-3\}$, one is able to obtain more complicated piece-wise C^∞-functions Φ_x in a similar fashion.

2.1.2. Test functions. In this thesis we consider several classes of test functions. The test functions are always of the form $h : \mathbb{K} \to \mathbb{C}$, where $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, and we always require that $h(0) = 0$. We now list the classes of test functions in ascending generality. We note that for increasing generality of the test functions we require more restrictive assumptions on the symbol in our proof of the Widom–Sobolev formula in Chapter 4.

The first class of studied test functions are polynomials. They will mostly play a role in the proof of intermediate results, which we then extend to one of the more general classes of test functions. We note that due to the assumption $h(0) = 0$, the constant part of the polynomial vanishes, and that, due to the linearity of the studied objects, the analysis reduces to monomial test functions. We usually denote the pth monomial, for $p \in \mathbb{N}$, by $g_p : \mathbb{C} \to \mathbb{C}$, with $g_p(z) := z^p$.

The next class of test functions we study, are analytic test functions. We require them to be analytic in a disc $B_R(0) \subseteq \mathbb{C}$ about the origin with sufficiently large radius $R > 0$, i.e. for $h : \mathbb{C} \to \mathbb{C}$ there exist $\omega_m \in \mathbb{C}, m \in \mathbb{N}$, such that

$$h(z) = \sum_{m \in \mathbb{N}} \omega_m z^m, \tag{2.4}$$

for all $z \in B_R(0)$. We again note the absence of ω_0, due to $h(0) = 0$. If we require the identity (2.4) to hold on the whole complex plane, we call h an entire function. The restriction to entire test functions is used to ease up the notation in some of the results, as we no longer need to worry about the specific radius $R > 0$.

We continue with smooth test functions $h : \mathbb{R} \to \mathbb{C}$ which we denote by $h \in C^\infty(\mathbb{R})$. We note that, as the domain of h already suggests, we only study these functions for self-adjoint arguments, where the application of the function is defined via the functional calculus.

The last and most general class of test functions studied is a bit less standard and characterised by the following

Assumption 2.5. Let $\gamma \in]0, 1]$ and let $\mathcal{X} := \{x_1, x_2, \ldots, x_N\} \subset \mathbb{R}, N \in \mathbb{N}$, be a finite collection of different points on the real line. Let $U_j \subset \mathbb{R}$, $j \in \{1, \ldots, N\}$, be pairwise disjoint neighbourhoods of the points $x_j \in \mathcal{X}$. Given a function $h \in C(\mathbb{R}) \cap C^2(\mathbb{R} \setminus \mathcal{X})$, we assume the existence of a constant $C > 0$ such that for every $k \in \{0, 1, 2\}$ the estimate

$$\left| \frac{\mathrm{d}^k}{\mathrm{d}x^k} \big[h - h(x_j) \big](x) \right| \leqslant C |x - x_j|^{\gamma - k}, \tag{2.5}$$

holds for every $x \in U_j \setminus \{x_j\}$ and every $j \in \{1, \ldots, N\}$. In particular, this implies that h is Hölder continuous at the points of $\mathcal{X}$.

Again we note that we only study the expression (2.1) for these test functions, if the corresponding operator is self-adjoint. One of the primary motivations to study these functions, is that they contain the Rényi entropy functions which we define in the following

Example 2.6. For a given parameter $\alpha \in]0, \infty[\setminus \{1\}$ the *Rényi entropy function* $h_\alpha : \mathbb{R} \to [0, \log 2]$ is given by

$$h_\alpha(t) := \frac{1}{1 - \alpha} \log[t^\alpha + (1 - t)^\alpha] \tag{2.6}$$

for $t \in [0,1]$ and by $h_\alpha(t) := 0$ elsewhere. Here log denotes the natural logarithm. In the case $\alpha = 1$ the *von Neumann entropy function* h_1 is given by

$$h_1(t) := \lim_{\alpha \to 1} h_\alpha(t) = -t \log t - (1-t)\log(1-t) \tag{2.7}$$

for $t \in]0,1[$ and by $h_1(t) := 0$ elsewhere. We note that $h_\alpha(0) = 0 = h_\alpha(1)$ for all $\alpha > 0$. The functions h_α satisfy Assumption 4.23 with $\gamma = \alpha$, for $\alpha \in]0,1[$, with arbitrary $\gamma \in]0,1[$, for $\alpha = 1$, and with $\gamma = 1$, for $\alpha \in]1,\infty[$.

2.1.3. Complex-valued symbols. The remaining objects which are yet to be explained in (2.1), are scalar-valued symbols and pseudo-differential operators corresponding to these symbols. We now give an introduction to these operators, to the extent that is required for the Widom–Sobolev formula. Afterwards, we give an overview of the Widom–Sobolev formula for scalar-valued symbols, proved in [Sob13, Sob14, Sob15, Sob17].

Given a natural number $d \in \mathbb{N}$, we consider *complex-valued amplitudes* $a \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d)$ which are smooth, i.e. arbitrarily often differentiable, and have the property that a and any partial derivative of a of arbitrary order is bounded. The first two variables of a play the role of space variables, the last one of a momentum variable. We denote the first variable by x, the second by y and the third by ξ. Given any such amplitude, the following integral formula defines a bounded [Cor75] linear operator on the Hilbert space $L^2(\mathbb{R}^d)$ of complex-valued square-integrable functions over $\mathbb{R}^d$, which leaves Schwartz space $\mathcal{S}(\mathbb{R}^d)$ invariant. Given a Schwartz function $u \in \mathcal{S}(\mathbb{R}^d)$, its action is defined by

$$\big(\mathrm{Op}_L^{lr}(a)u\big)(x) := \left(\frac{L}{2\pi}\right)^d \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}L\xi(x-y)}\, a(x,y,\xi)u(y)\,\mathrm{d}y\,\mathrm{d}\xi \tag{2.8}$$

for every $x \in \mathbb{R}^d$. Here, i denotes the imaginary unit, and the integrations are with respect to Lebesgue measure in $\mathbb{R}^d$. In the case that the function a does not depend on both x and y, we call a a *complex-valued symbol* and define the left and right operators of a by

$$\big(\mathrm{Op}_L^{l}(a)u\big)(x) := \left(\frac{L}{2\pi}\right)^d \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}L\xi(x-y)}\, a(x,\xi)u(y)\,\mathrm{d}y\,\mathrm{d}\xi \tag{2.9}$$

and

$$\big(\mathrm{Op}_L^{r}(a)u\big)(x) := \left(\frac{L}{2\pi}\right)^d \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}L\xi(x-y)}\, a(y,\xi)u(y)\,\mathrm{d}y\,\mathrm{d}\xi. \tag{2.10}$$

If a depends only on ξ, we no longer need the distinction between left and right operators and just write $\mathrm{Op}_L(a)$. In this case, we have

$$\mathrm{Op}_L(a) = \mathcal{F}^{-1} a(\cdot/L)\mathcal{F}, \tag{2.11}$$

where $\mathcal{F}$ is the unitary Fourier transform on $L^2(\mathbb{R}^d)$ and, on the right-hand side, a is to be understood as a multiplication operator (in Fourier space). Thus, in the case of (2.11), $\mathrm{Op}_L(a)$ gives rise to a well-defined and bounded operator on $L^2(\mathbb{R}^d)$, whenever the symbol a is an essentially bounded measurable function on $\mathbb{R}^d$.

In order to obtain (2.1), we introduce discontinuities in both variables x and ξ of the left operator of the symbol a. Let $\Lambda, \Gamma \subseteq \mathbb{R}^d$ be bounded measurable subsets. Then we define the following operator on $L^2(\mathbb{R}^d)$

$$T_L(a) := T_L(a;\Lambda,\Gamma) := 1_\Lambda\, \mathrm{Op}_L(1_\Gamma)\, \mathrm{Op}_L^l(a)\, \mathrm{Op}_L(1_\Gamma) 1_\Lambda, \tag{2.12}$$

where 1_Λ, 1_Γ are the associated indicator functions, 1_Λ acts as a multiplication operator and $\mathrm{Op}_L(1_\Gamma)$ is defined by (2.11). The operator $\mathrm{Op}_L(1_\Gamma)1_\Lambda$ is trace class according to [BS87, Chap. 11, Sect. 8, Thm. 11]. Therefore, T_L and its symmetrised version

$$S_L(a) := S_L(a;\Lambda,\Gamma) := 1_\Lambda \,\mathrm{Op}_L(1_\Gamma)\,\mathrm{Re}\left[\mathrm{Op}_L^l(\mathrm{Re}\,a)\right]\mathrm{Op}_L(1_\Gamma)1_\Lambda, \tag{2.13}$$

which is self-adjoint and has a real-valued symbol, are both trace class. Here, we denote by Re the self-adjoint part $\mathrm{Re}\,Q := (Q+Q^*)/2$ of a bounded operator Q.

We now have all the required prerequisites to state the asymptotic expansion of the Widom–Sobolev formula for scalar-valued symbols. Let $a \in C_b^\infty(\mathbb{R}^d)$ be a scalar-valued symbol. Then the asymptotic expansion

$$\begin{aligned}\mathrm{tr}_{L^2(\mathbb{R}^d)}\left[h\big(S_L(a)\big)\right] = L^d\mathfrak{W}_0\big(h(\mathrm{Re}\,a);\Lambda,\Gamma\big) + L^{d-1}\log L\; \mathfrak{W}_1\big(\mathfrak{U}(h;\mathrm{Re}\,a);\partial\Lambda,\partial\Gamma\big)\\ + o(L^{d-1}\log L)\end{aligned} \tag{2.14}$$

holds for suitable test functions $h:\mathbb{R}\longrightarrow\mathbb{R}$ with $h(0)=0$ as $L\longrightarrow\infty$. This was proved by A.V. Sobolev in [Sob13, Sob15] for analytic and smooth test functions and extended in [Sob14, Sob17] to test functions satisfying Assumption 2.5, under the assumption that the symbol a only depends on the variable ξ. In all three cases, Λ is required to be a bounded piece-wise C^1-admissible domain and Γ is required to be a bounded piece-wise C^3-admissible domain. The coefficients are given, for continuous symbols b, by

$$\mathfrak{W}_0(b;\Lambda,\Gamma) := \frac{1}{(2\pi)^d}\int_\Lambda\int_\Gamma b(x,\xi)\,\mathrm{d}\xi\,\mathrm{d}x \tag{2.15}$$

and

$$\mathfrak{W}_1(b;\partial\Lambda,\partial\Gamma) := \begin{cases}\displaystyle\sum_{(x,\xi)\in\partial\Lambda\times\partial\Gamma} b(x,\xi), & \text{for } d=1,\\ \displaystyle\frac{1}{(2\pi)^{d-1}}\int_{\partial\Lambda}\int_{\partial\Gamma} b(x,\xi)\,|\nu_{\partial\Lambda}(x)\cdot\nu_{\partial\Gamma}(\xi)|\,\mathrm{d}S(\xi)\,\mathrm{d}S(x), & \text{for } d\geqslant 2,\end{cases} \tag{2.16}$$

where $\nu_{\partial\Lambda}$, respectively $\nu_{\partial\Gamma}$, denotes the vector field of exterior unit normals in $\mathbb{R}^d$ to the boundary $\partial\Lambda$, respectively $\partial\Gamma$. We write $\mathrm{d}S$ for integration with respect to the $(d-1)$-dimensional surface measure induced by Lebesgue measure in $\mathbb{R}^d$. Finally, the symbol $\mathfrak{U}(g;b)$ in (2.14) is given by

$$\mathfrak{U}(g;b)(x,\xi) := \frac{1}{(2\pi)^2}\int_0^1 \frac{g\big(tb(x,\xi)\big)-tg\big(b(x,\xi)\big)}{t(1-t)}\,\mathrm{d}t \tag{2.17}$$

for every $x,\xi\in\mathbb{R}^d$ and for Hölder-continuous test functions g.

Remark 2.7. In the case of analytic or smooth test functions, the above asymptotics (2.14) holds for a more general class of symbols which are not required to be arbitrarily often differentiable but merely have a finite symbol norm $\mathbf{N}^{(m_x,m_\xi)}(a)$ for $m_x = m_\xi = d+2$. For the definition of the symbol norm, we refer to Definition 2.8 below with $n=1$. If the test function h only satisfies Assumption 2.5, which is relevant for applications, the required parameter m_ξ in the norm increases significantly. This is the reason for the restriction onto smooth symbols in the present section and Chapters 3 and 4. This minimises some technical notation and allows us to focus on aspects more relevant to our application in Chapter 5, like the possible choices for the domain Γ.

2.1.4. Matrix-valued symbols. With all the prerequisites for the known scalar case being established, we now turn to matrix-valued symbols and the results we prove in Chapter 4.

Given a complex square matrix $A \in \mathbb{C}^{n\times n}$ with matrix dimension $n \in \mathbb{N}$, we denote its entry in the νth row and μth column by $(A)_{\nu\mu}$, where $\nu, \mu \in \{1, \ldots, n\}$. We now introduce *matrix-valued amplitudes* $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ which are arbitrarily often differentiable and have the property that A and any partial derivative of A of arbitrary order is bounded. We will always identify this space with the tensor product

$$C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n}) = C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d) \otimes \mathbb{C}^{n\times n}. \tag{2.18}$$

Thus, $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ is equivalent to requiring that the matrix entries of A are corresponding complex-valued amplitudes, i.e. $(A)_{\nu\mu} \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d)$ for any $\nu, \mu \in \{1, \ldots, n\}$. If $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ does not depend on both x and y, we call A a *matrix-valued symbol*.

In analogy to the scalar case, we define bounded – see Lemma 3.1 – matrix-valued operators $\mathrm{Op}_L^{lr}(A), \mathrm{Op}_L^{l}(A)$ and $\mathrm{Op}_L^{r}(A)$ on the product Hilbert space $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$. Their action on Schwartz functions $u \in \mathcal{S}(\mathbb{R}^d) \otimes \mathbb{C}^n$ is given by

$$\big(\mathrm{Op}_L^{lr}(A)u\big)(x) := \left(\frac{L}{2\pi}\right)^d \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}L\xi(x-y)}\, A(x,y,\xi)u(y)\mathrm{d}y\mathrm{d}\xi, \tag{2.19}$$

$$\big(\mathrm{Op}_L^{l}(A)u\big)(x) := \left(\frac{L}{2\pi}\right)^d \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}L\xi(x-y)}\, A(x,\xi)u(y)\mathrm{d}y\mathrm{d}\xi \tag{2.20}$$

and

$$\big(\mathrm{Op}_L^{r}(A)u\big)(x) := \left(\frac{L}{2\pi}\right)^d \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}L\xi(x-y)}\, A(y,\xi)u(y)\mathrm{d}y\mathrm{d}\xi, \tag{2.21}$$

for every $x \in \mathbb{R}^d$. We write $\mathrm{Op}_L(A)$, if A only depends on the variable ξ. In this case, we have

$$\mathrm{Op}_L(A) = (\mathcal{F}^{-1} \otimes \mathbb{1}_n)\, A(\,\cdot/L)\, (\mathcal{F} \otimes \mathbb{1}_n), \tag{2.22}$$

where, on the right-hand side, A is to be understood as a multiplication operator in $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$. Thus, in the case of (2.22), $\mathrm{Op}_L(A)$ gives rise to a well-defined and bounded operator on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$, whenever the symbol A is an essentially bounded measurable matrix-valued function on $\mathbb{R}^d$.

In the analysis carried out in Chapters 3 - 5, we sometimes need to control bounds depending on the size of support and decay of a given amplitude or symbol. For these cases, we define the following symbol norm.

Definition 2.8. Given non-negative integers $m_x, m_y, m_\xi \in \mathbb{N}_0$, real number $s, \tau > 0$ and a matrix-valued amplitude $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$, we introduce the *symbol norm*

$$\mathbf{N}^{(m_x,m_y,m_\xi)}(A; s, \tau) := \max_{\substack{|\alpha|\leqslant m_x\\ |\beta|\leqslant m_y\\ |\gamma|\leqslant m_\xi}} \sup_{x,y,\xi\in\mathbb{R}^d} s^{m_x+m_y}\tau^{m_\xi}\, \mathrm{tr}_{\mathbb{C}^n} \left|\partial_x^\alpha \partial_y^\beta \partial_\xi^\gamma A(x,y,\xi)\right| < \infty \tag{2.23}$$

of A. Here, $\alpha, \beta, \gamma \in \mathbb{N}_0^d$ are multi-indices, $|\alpha| := \sum_{j=1}^d |\alpha_j|$ and $\partial_u^\alpha := \frac{\partial^{|\alpha|}}{\partial_{u_1}^{\alpha_1}\cdot\ldots\cdot\partial_{u_d}^{\alpha_d}}$, where ∂_{u_j} denotes the partial derivative with respect to the jth component of the variable $u \in \mathbb{R}^d$. If $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ is a matrix-valued symbol which does not depend on the variable y, respectively x, we set $\mathbf{N}^{(m_x,m_\xi)}(A; s, \tau) := \mathbf{N}^{(m_x,m_y,m_\xi)}(A; s, \tau)$ for arbitrary m_y, respectively $\mathbf{N}^{(m_y,m_\xi)}(A; s, \tau) := \mathbf{N}^{(m_x,m_y,m_\xi)}(A; s, \tau)$ for arbitrary m_x. Sometimes, we do not require the dependence on the parameters s and τ. Then we write $\mathbf{N}^{(m_x,m_y,m_\xi)}(A) := \mathbf{N}^{(m_x,m_y,m_\xi)}(A; 1, 1)$.

The indicator functions of the bounded measurable subsets $\Lambda, \Gamma \subset \mathbb{R}^d$ on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$ are given by

$$\mathbf{1}_\Lambda := 1_\Lambda \otimes \mathbb{1}_n; \qquad \mathbf{1}_\Gamma := 1_\Gamma \otimes \mathbb{1}_n, \tag{2.24}$$

where the respective second factor denotes the $n \times n$-unit matrix. We also introduce operators induced by matrix-valued symbols $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ with discontinuities in both variables

$$T_L(A) := T_L(A; \Lambda, \Gamma) := \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Op}_L^l(A) \operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda \tag{2.25}$$

and

$$S_L(A) := S_L(A; \Lambda, \Gamma) := \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Re}\big[\operatorname{Op}_L^l(\operatorname{Re} A)\big] \operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda, \tag{2.26}$$

where we employ the same notation as in the scalar cases (2.12) and (2.13).

It is useful to reduce the traces of these operators, to the traces of operators with scalar-valued symbols. For $\nu, \mu \in \{1, \dots, n\}$, let $E_{\nu\mu} \in \mathbb{C}^{n\times n}$ be the canonical matrix unit with entry one in the νth row and μth column and all other entries equal to zero. We expand the matrix-valued symbol A with respect to this matrix basis

$$A = \sum_{\nu,\mu=1}^{n} (A)_{\nu\mu} \otimes E_{\nu\mu} \tag{2.27}$$

and use linearity to obtain

$$T_L(A) = \sum_{\nu,\mu=1}^{n} T_L\big((A)_{\nu\mu} \otimes E_{\nu\mu}\big) = \sum_{\nu,\mu=1}^{n} T_L\big((A)_{\nu\mu}\big) \otimes E_{\nu\mu}. \tag{2.28}$$

Given a trace-class operator T on $L^2(\mathbb{R}^d)$ and a matrix $M \in \mathbb{C}^{n\times n}$, their elementary tensor product $T \otimes M$ is trace class on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$ with (standard) trace $\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} T \otimes M = (\operatorname{tr}_{L^2(\mathbb{R}^d)} T)(\operatorname{tr}_{\mathbb{C}^n} M)$. In particular, the operator $T_L(A)$ is trace class with

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} T_L(A) = \sum_{\nu=1}^{n} \operatorname{tr}_{L^2(\mathbb{R}^d)} T_L\big((A)_{\nu\nu}\big) = \operatorname{tr}_{L^2(\mathbb{R}^d)}[T_L(\operatorname{tr}_{\mathbb{C}^n} A)], \tag{2.29}$$

where we interpret $\operatorname{tr}_{\mathbb{C}^n} A : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$ as a complex-valued symbol. In the same way, the operator $S_L(A)$ is seen to be trace class.

Motivated by the applications to the free Dirac operator in Chapter 5, it will be useful to extend the asymptotic formula to slightly more general Wiener–Hopf operators which are not only restricted to the momentum region $\Gamma \subset \mathbb{R}^d$ as in (2.25) and (2.26) but, instead, exhibit a more general jump discontinuity at the boundary $\partial\Gamma$ with different matrix-valued symbols $A_1, A_2 \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ on the inside, respectively outside of $\partial\Gamma$. Since at least one of the domains Γ and Γ^c is not bounded we require the symbols A_1, respectively A_2, to be compactly supported in the second variable, when Γ, respectively Γ^c, is not bounded. This guarantees the trace-class property of the operators

$$D_L(A_1, A_2) := D_L(A_1, A_2; \Lambda, \Gamma) := T_L(A_1; \Lambda, \Gamma) + T_L(A_2; \Lambda, \Gamma^c) \tag{2.30}$$

and

$$G_L(A_1, A_2) := G_L(A_1, A_2; \Lambda, \Gamma) := S_L(A_1; \Lambda, \Gamma) + S_L(A_2; \Lambda, \Gamma^c). \tag{2.31}$$

In this case, we also need to adapt the symbol $\mathfrak{U}(g; b)$ in (2.17) featuring in the $\mathfrak{W}_1$-coefficient to account for both A_1 and A_2. Similarly to the situation in $d = 1$ dimension for matrix-valued symbols with general jump discontinuities in [Wid82], the appropriate replacement appearing in Theorem 2.9 is

$$\mathfrak{U}(g; B_1, B_2) := \frac{1}{(2\pi)^2} \int_0^1 \frac{\operatorname{tr}_{\mathbb{C}^n}\big[g\big(B_1 t + B_2(1-t)\big) - g(B_1)t - g(B_2)(1-t)\big]}{t(1-t)}\, \mathrm{d}t \tag{2.32}$$

which is defined for bounded matrix-valued symbols B_1, B_2 and for Hölder continuous functions $g : \mathbb{R} \to \mathbb{C}$.

With the required objects and notation at hand, we are now able to state our Widom–Sobolev formula for matrix-valued symbols, the main result of Chapter 4. We note that the following version is slightly simplified in several places to avoid cumbersome notation and in Chapter 4 the result is split into several different theorems, corresponding to the strategy of the proof.

Theorem 2.9. *Let $A_1, A_2 \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be matrix-valued symbols. Let Λ be a bounded piece-wise C^1-admissible domain and Γ be a piece-wise C^3-admissible domain. Let $X \in \{D, G\}$. If at least one of the assumptions*

- *($\mathcal{A}1$) the function h is analytic in a disc of sufficiently large radius with $h(0) = 0$;*
- *($\mathcal{A}2$) the function $h \in C^\infty(\mathbb{R})$ is smooth with $h(0) = 0$ and $X = G$;*
- *($\mathcal{A}3$) the function satisfies Assumption 2.5 with $h(0) = 0$, we have $X = G$ and the symbols A_1 and A_2 only depend on the single variable ξ;*

and at least one of the assumptions

- *($\mathcal{B}1$) the domain Γ is bounded and A_2 is compactly supported in the second variable;*
- *($\mathcal{B}2$) the domain Γ^c is bounded and A_1 is compactly supported in the second variable;*
- *($\mathcal{B}3$) both the symbols A_1 and A_2 are compactly supported in the second variable;*

is fulfilled, the following asymptotic formula holds

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(X_L(A_1, A_2; \Lambda, \Gamma)\big)\big] &= L^d\Big(\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(A_1)]; \Lambda, \Gamma\big) + \mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(A_2)]; \Lambda, \Gamma^c\big)\Big)\\ &\quad + L^{d-1}\log L\ \mathfrak{W}_1\big(\mathfrak{U}(h; A_1, A_2); \partial\Lambda, \partial\Gamma\big)\\ &\quad + o(L^{d-1}\log L),\end{aligned} \tag{2.33}$$

as $L \to \infty$. Here, the coefficients $\mathfrak{W}_0$ and $\mathfrak{W}_1$ were defined in (2.15) *and* (2.16)*, respectively, and the symbol $\mathfrak{U}$ in* (2.32)*.*

2.2. Application to the free Dirac Operator

The self-adjoint Hamiltonian of the Dirac equation in $d \in \mathbb{N}$ space dimensions is given by

$$D := -\mathrm{i}\sum_{k=1}^{d}\alpha_k\partial_k + m\beta, \tag{2.34}$$

see e.g. [Dan00, KY01]. It is densely defined in the product Hilbert space $L^2(\mathbb{R}^d) \otimes \mathbb{C}^{n_d}$ of square-integrable vector-valued functions with spinor dimension $n_d := 2^{\lfloor (d+1)/2\rfloor}$. Here, $\lfloor r\rfloor$ stands for the largest integer not exceeding $r \in \mathbb{R}$. Moreover, i is the imaginary unit, $m \geqslant 0$ is the mass of the particle, ∂_k, $k = 1, \dots, d$, denotes partial differentiation with respect to the kth Cartesian coordinate and $\beta, \alpha_1, \dots, \alpha_d \in \mathbb{C}^{n_d\times n_d}$ are Dirac matrices which anti-commute pairwise and whose square gives the $n_d \times n_d$-unit matrix $\mathbb{1}_{n_d}$. As shown by A. Hurwitz [Hur22], the number $n_d = 2^{\lfloor (d+1)/2\rfloor}$ is the smallest natural number such that $d + 1$ such matrices exist. The choice of Dirac matrices is then unique up to similarity transformations. As the trace is invariant under such transformations, the results of this thesis are, for the given choice of n_d, independent of the choice of Dirac matrices.

The Dirac matrices can be chosen as (cf. [Hur22] resp. [KY01, Appendix])

$$\alpha_j := \begin{pmatrix} 0 & \sigma_j \\ \sigma_j^* & 0 \end{pmatrix}, \quad j = 1, \dots, d, \quad \text{and} \quad \beta := \begin{pmatrix} \mathbb{1}_{\frac{n_d}{2}} & 0 \\ 0 & -\mathbb{1}_{\frac{n_d}{2}} \end{pmatrix}, \tag{2.35}$$

where the $\frac{n_d}{2} \times \frac{n_d}{2}$-matrices σ_j satisfy the anti-commutation relations

$$\sigma_j \sigma_k^* + \sigma_k \sigma_j^* = 2\delta_{jk} \mathbb{1}_{\frac{n_d}{2}} \quad \text{and} \quad \sigma_j^* \sigma_k + \sigma_k^* \sigma_j = 2\delta_{jk} \mathbb{1}_{\frac{n_d}{2}} \tag{2.36}$$

for all $j, k = 1, \ldots, d$. In the case that d is odd, the matrices σ_j are Hermitian for all $j = 1, \ldots, d$. In (2.36), $*$ denotes the adjoint and $\delta_{jk} := 1$ if $j = k$ and 0 otherwise the Kronecker delta. In particular, we immediately see that the Dirac matrices α_k, $k \in \{1, \ldots, d\}$, and β are Hermitian with vanishing trace. For the remaining part of the present thesis it is convenient to drop the subscript d for the spinor dimension n_d, i.e. we write $n = n_d$

The Hamiltonian given in (2.34) is unitarily equivalent via the Fourier transform to the operator of multiplication on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^{n \times n}$ with the (unbounded) matrix-valued symbol

$$\mathbb{R}^d \ni \xi = (\xi_1, \ldots, \xi_d) \mapsto D(\xi) := \sum_{k=1}^{d} \alpha_k \xi_k + m\beta, \tag{2.37}$$

see, for example, [Tha92]. Clearly, the symbol D is smooth, i.e. $D \in C^\infty(\mathbb{R}^d, \mathbb{C}^{n \times n})$. We note that we use the same letter D for both the Hamiltonian in (2.34) and the symbol in (2.37). Still, it will always be clear from the context which of the objects we refer to.

We want to study the application of measurable functions to this operator. In order to do so, it is convenient to diagonalise the matrix $D(\xi)$ at every possible point $\xi \in \mathbb{R}^d$ in momentum space. We first note that the matrix $D(\xi)$ is regular except in the case $\xi = 0$, $m = 0$, where $D(\xi) = 0$. Using the anti-commutation relations (2.36), we see that $D^2(\xi) = E^2(\xi)\mathbb{1}_n$, where $E : \mathbb{R}^d \to [0, \infty[$ is the relativistic energy momentum relation given by

$$E(\xi) := \sqrt{m^2 + \xi^2}. \tag{2.38}$$

We further note that the matrix $D(\xi)$ has vanishing trace as a sum of matrices with vanishing trace and is Hermitian. Therefore, the matrix $D(\xi)$ has both $E(\xi)$ and $-E(\xi)$ as eigenvalues of multiplicity $\frac{n}{2}$ and, in the case $E(\xi) \neq 0$, it can be diagonalised as

$$U(\xi) D(\xi) U^{-1}(\xi) = E(\xi)\beta, \tag{2.39}$$

where $U(\xi)$ is a unitary matrix. We now calculate $a(D(\xi))$ for some measurable function $a : \mathbb{R} \to \mathbb{C}$. Using the diagonalisation above, we obtain

$$a\big(D(\xi)\big) = a\big(U^{-1}(\xi)E(\xi)\beta U(\xi)\big) = U^{-1}(\xi) a\big(E(\xi)\beta\big) U(\xi). \tag{2.40}$$

The matrix $a\big(E(\xi)\beta\big)$ is diagonal with entries $a\big(E(\xi)\big)$ and $a\big(-E(\xi)\big)$. We define two functions $a_\pm$ on momentum space by

$$a_+(\xi) := a\big(E(\xi)\big), \qquad a_-(\xi) := a\big(-E(\xi)\big). \tag{2.41}$$

Then we write (2.40) as

$$\begin{aligned} a\big(D(\xi)\big) = U^{-1}(\xi) a\big(E(\xi)\beta\big) U(\xi) &= \frac{1}{2} U^{-1}(\xi) \Big((a_+ + a_-)(\xi) \mathbb{1}_n + (a_+ - a_-)(\xi)\beta \Big) U(\xi) \\ &= \frac{1}{2}(a_+ + a_-)(\xi)\mathbb{1}_n + \frac{1}{2}(a_+ - a_-)(\xi) \frac{D}{E}(\xi) \end{aligned} \tag{2.42}$$

for every $\xi \in \mathbb{R}^d$, where we define $\frac{D}{E}(0) := 0$ in the case $m = 0$.

We now remark on some properties of the symbol $a(D)$ stemming from the equality above and view the operator $a(D)$ in the context of Section 2.1.

Remark 2.10. (a) In order for the notation in (2.42) to be sensible, we identify the matrix $\mathbb{1}_n$ with a constant matrix-valued symbol. The multiplication of a scalar-valued symbol with a matrix-valued symbol is defined point-wise by scalar multiplication on the tensor product. These notational conventions will be used extensively throughout the thesis.

(b) If the function a in (2.42) is (essentially) bounded, the symbol $a(D)$ is also (essentially) bounded. Then, for every $L > 0$, the operator $\mathrm{Op}_L(a(D))$ extends to a well-defined and bounded operator on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$, in the sense of Section 2.1.4. We then write the application of the function a to the Hamiltonian D as the operator with matrix-valued symbol $a(D)$, i.e. $a(D) = \mathrm{Op}_1(a(D))$.

(c) If the function a in (2.42) is compactly supported, the functions a_+ and a_- are also compactly supported. Therefore, the symbol $a(D)$ is compactly supported in this case.

(d) If there exists $\tilde{a} : \mathbb{R} \to \mathbb{C}$ measurable such that its support satisfies $\operatorname{supp}(a - \tilde{a}) \subseteq [-m, m]$, then, by virtue of (2.42), the equality $\tilde{a}(D) = a(D)$ holds Lebesgue-almost everywhere, in particular we have $\mathrm{Op}_L\left(\tilde{a}(D)\right) = \mathrm{Op}_L\left(a(D)\right)$.

(e) If the function a in (2.42) is smooth on the range of the positive and negative energy function $\operatorname{ran} \pm E = \,]-\infty, -m] \cup [m, \infty[$ (at the boundaries to be understood as one-sided derivatives), then the functions a_+ and a_- are smooth on $\mathbb{R}^d$. In this case, the symbol $a(D)$ is smooth if $m > 0$, as this guarantees smoothness of the symbol $\frac{D}{E}$ on $\mathbb{R}^d$. If $m = 0$, the additional assumption $a(0) = 0$ also implies smoothness of $a(D)$ despite the discontinuity of the symbol $\frac{D}{E}$ at the origin.

For the application to the free Dirac operator, we study the symbol $\chi_{E_F}^{(b)}(D)$, where $\chi_{E_F}^{(b)}$ is the following smoothly truncated version of the Fermi projection. Given a Fermi energy $E_F \in \mathbb{R}$ and an ultraviolet cut-off parameter $b \in [0, \infty[$, we define

$$\chi_{E_F}^{(b)} : \mathbb{R} \to [0, 1], \quad x \mapsto \chi_{E_F}^{(b)}(x) := 1_{\{y \in \mathbb{R} : y < E_F\}}(x) \varphi_{E_F}(x + b) \tag{2.43}$$

in terms of the monotone cut-off function $\varphi_{E_F} := \varphi \in C^\infty(\mathbb{R})$ obeying $\varphi|_{[-|E_F|, \infty[} = 1$ and $\varphi|_{]-\infty, -|E_F|-1]} = 0$. We note that the function $\chi_{E_F}^{(b)}$ is bounded and compactly supported.

2.2.1. Relation to the entanglement entropy and main results. In our application to the free Dirac operator, we restrict ourselves to the general case of test functions which satisfy Assumption 2.5. The reason for this is twofold. On the one hand, studying the free Dirac operator makes this possible, as the symbol $\chi_{E_F}^{(b)}(D)$ is only supported in the single variable ξ. On the other hand, these functions include the Rényi entropy functions, see Section 2.1.

The Rényi entropy functions are of particular interest here, as, for $\alpha \in]0, \infty[$, the trace

$$\operatorname{tr}_{L^2(\mathbb{R}^d) \otimes \mathbb{C}^n} \left[h_\alpha\left(\mathbf{1}_\Omega \chi_{E_F}^{(b)}(D) \mathbf{1}_\Omega\right) \right] \tag{2.44}$$

corresponds to the bipartite α-Rényi entropy, with respect to the domain $\Omega \subset \mathbb{R}^d$, of an ensemble of non-interacting particles which are all described by the same single-particle Hamiltonian – the free Dirac operator. This type of correspondence, in the case that the single-particle Hamiltonian is not given by the free Dirac operator but the Laplacian, i.e. the free Schrödinger operator, was first observed in [GK06] and is based on the analysis in [Kli06].

We now formulate the main object studied in Chapter 5. Let $\Lambda, \Lambda' \subset \mathbb{R}^d$ with $\Lambda \subset \Lambda'$ be bounded piece-wise C^1-admissible domains. Given a subset $\Omega \subseteq \mathbb{R}^d$ and $L > 0$, we introduce the scaled subset $\Omega_L := \{Lx \in \mathbb{R}^d : x \in \Omega\}$. We study the following trace

$$\operatorname{tr}_{L^2(\mathbb{R}^d) \otimes \mathbb{C}^n} \left[h\left(\mathbf{1}_{\Lambda_L} \chi_{E_F}^{(b)}(D) \mathbf{1}_{\Lambda_L}\right) + h\left(\mathbf{1}_{\Lambda'_L \setminus \Lambda_L} \chi_{E_F}^{(b)}(D) \mathbf{1}_{\Lambda'_L \setminus \Lambda_L}\right) - h\left(\mathbf{1}_{\Lambda'_L} \chi_{E_F}^{(b)}(D) \mathbf{1}_{\Lambda'_L}\right) \right], \tag{2.45}$$

for fixed Fermi energy $E_F \in \mathbb{R}$, mass $m \geqslant 0$ and energy cut-off $b \geqslant 0$. We recall that $\mathbf{1}_\Omega = 1_\Omega \otimes \mathbb{1}_n$ acts as the multiplication operator by the corresponding matrix-valued indicator function on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$.

As all of the domains Λ, Λ', $\Lambda' \setminus \Lambda$ are bounded and the function $\chi_{E_F}^{(b)}$ is compactly supported, all the operators in (2.45) are trace class, see [BS87, Chap. 11, Sect. 8, Thm. 11].

The advantage of studying a difference as in (2.45) is that the leading term of order L^d cancels out. If the function h is chosen to be one of the Rényi entropy functions, the trace (2.45) is related to the relative local Rényi entropy corresponding to the domains Λ and Λ'.

Our main result, regarding the application to the free Dirac operator, is the following asymptotic expansion of the trace (2.45). Here, we split the analysis into several cases, depending on both the mass m and the Fermi energy E_F. In some cases we obtain an enhanced area law and in other cases we show that at most an area law can hold.

Theorem 2.11. *Let $\Lambda \subset \Lambda'$ be bounded piece-wise C^1-admissible domains in $\mathbb{R}^d$ in the sense of Definition 2.2 and such that $\operatorname{dist}(\Lambda, \partial\Lambda') > 0$. Consider the Dirac operator (2.34) with mass $m \geqslant 0$ and fix a Fermi energy $E_F \in \mathbb{R}$ and an ultraviolet cut-off parameter $b \geqslant 0$. Let $h \in C(\mathbb{R})$ satisfy Assumption 4.23 and $h(0) = 0$. Then the asymptotic trace formula*

$$\frac{1}{n} \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \Big[h\big(\mathbf{1}_{\Lambda_L} \chi_{E_F}^{(b)}(D) \mathbf{1}_{\Lambda_L}\big) + h\big(\mathbf{1}_{\Lambda'_L\setminus\Lambda_L} \chi_{E_F}^{(b)}(D) \mathbf{1}_{\Lambda'_L\setminus\Lambda_L}\big) - h\big(\mathbf{1}_{\Lambda'_L} \chi_{E_F}^{(b)}(D) \mathbf{1}_{\Lambda'_L}\big) \Big]$$
$$= L^{d-1} \log L \; W(h, \Lambda, E_F, m) + o(L^{d-1}\log L) \quad (2.46)$$

holds as $L \to \infty$. The coefficient $W(h, \Lambda, E_F, m)$ is independent of the cut-off parameter b, the domain Λ' and the spinor dimension n. Moreover:

(a) *If $|E_F| > m$, then the coefficient of this enhanced area law is given by*

$$W(h, \Lambda, E_F, m) := \frac{\Phi(\Lambda, E_F, m)}{(2\pi)^2} \int_0^1 \frac{h(t) - h(1)t}{t(1-t)} \,\mathrm{d}t \quad (2.47)$$

with the geometric factor

$$\Phi(\Lambda, E_F, m) := \begin{cases} 2|\partial\Lambda|, & \text{if } d = 1, \\ \dfrac{1}{(2\pi)^{d-1}} \displaystyle\int_{\partial\Lambda} \int_{\partial B_{p_F}} |\nu_{\partial\Lambda}(x) \cdot \nu_{\partial B_{p_F}}(\xi)| \,\mathrm{d}S(\xi)\mathrm{d}S(x), & \text{if } d \geqslant 2, \end{cases} \quad (2.48)$$

where, in one dimension, $|\partial\Lambda|$ is the number of boundary points of Λ. In dimensions $d \geqslant 2$, we write $B_{p_F} := B_{p_F}(0)$, where $p_F := \sqrt{E_F^2 - m^2}$ is the relativistic Fermi momentum, and $\nu_{\partial\Lambda}$, resp. $\nu_{\partial B_{p_F}}$, denotes the vector field of exterior unit normals in $\mathbb{R}^d$ to $\partial\Lambda$, resp. ∂B_{p_F}. We write $\mathrm{d}S$ for integration with respect to the $(d-1)$-dimensional surface measure induced by Lebesgue measure in $\mathbb{R}^d$.

(b) *If $|E_F| \leqslant m \neq 0$, then $W(h, \Lambda, E_F, m) = 0$, and the next term in the asymptotic expansion is of order $O(L^{d-1})$ as $L \to \infty$.*

(c) *If $E_F = m = 0$, then the behaviour depends on the dimension. If $d = 1$ an enhanced area law holds with the same coefficient (5.5) and (5.6) as in (a). If instead $d \geqslant 2$, the situation is as in (b).*

2.3. Lower-order terms in the massless case

2.3.1. The free massless Dirac Operator. We now turn towards the special case $E_F = m = 0$ of the operator studied in Section 2.2. Therefore, we take a closer look at the symbol $\chi_0^{(b)}(D)$. Here, the function $\chi_0^{(b)}$ is defined in (2.43). The application of such a function to D has already been studied in Section 2.2, in the more general case with non-negative mass m and arbitrary Fermi energy

$E_F \in \mathbb{R}$. In the special case $E_F = m = 0$, the energy, as a function on momentum space, is given by $E(\xi) := |\xi|$ and by (2.42) the symbol of the operator $\chi_0^{(b)}(D)$ is given by

$$\big(\chi_0^{(b)}(D)\big)(\xi) = \psi^{(b)}(\xi)\tfrac{1}{2}\big(\mathbb{1}_n - \tfrac{D}{E}(\xi)\big) = \psi^{(b)}(\xi)\tfrac{1}{2}\Big(\mathbb{1}_n - \sum_{k=1}^{d} \alpha_k \tfrac{\xi_k}{|\xi|}\Big) =: \psi^{(b)}(\xi)\mathcal{D}(\xi), \qquad (2.49)$$

where $\psi(\xi) := \psi^{(b)}(\xi) := \varphi(-E(\xi) + b)$ for every $\xi \in \mathbb{R}^d$ and we define $\frac{D}{E}(0) := 0$. The symbol $\psi^{(b)}$ is smooth and compactly supported in the ball $B_{b+1}(0)$ of radius $b+1$ centred about the origin, and satisfies $\|\psi^{(b)}\|_\infty = 1$. The symbol $\mathcal{D}$ is discontinuous precisely at the origin and smooth everywhere else.

As seen in Theorem 2.9, this zero-dimensional discontinuity is not sufficient to lead to an enhanced area law. In fact, it seems similar to the case $|E_F| \leqslant m \neq 0$, where the symbol does not feature any discontinuity. The difference of these cases only becomes apparent, when one also studies the lower-order terms of the expansion. For sufficiently smooth symbols, several multi-term, or even complete, asymptotic expansions are known, for suitable domains, see e.g. [Roc84, Wid85, Die18, Pfi19]. It is certainly feasible, although it is not the content of this thesis, to also obtain similar expansions in the case $|E_F| \leqslant m \neq 0$ of Theorem 2.9, where the symbol is effectively smooth.

The motivation behind the results contained in Chapter 6 is to show that the asymptotic expansion in the case $E_F = m = 0$ differs from the one for smooth symbols precisely starting at the $(d+1)$st term. Instead of a constant term in the smooth case, a lower order enhanced term of order $\log L$ follows. One way to explain this behaviour from a mathematical point of view, is the fact that the discontinuity at the origin of the symbol $\mathcal{D}$ leads to significantly worse decay of the integral kernel K of the corresponding operator. We take a closer look at this decay in Chapter 6. As in the already established results on multi-term asymptotic expansions, we further restrict our choice of domain Λ, acting as a spatial restriction. Due to the zero-dimensional discontinuity of the symbol $\mathcal{D}$, we are particularly interested in domains which feature "corners", i.e. isolated points where the smoothness of the boundary $\partial\Lambda$ breaks down. In order to both consider domains with only piece-wise smooth boundary and keep the ensuing analysis manageable, we restrict ourselves to the special case of a d-dimensional cube as in [Die18].

2.3.2. Main results. In this section and Chapter 6, we restrict ourselves to entire test functions $h : \mathbb{C} \to \mathbb{C}$ which satisfy $h(0) = 0$. The assumption that the functions are analytic on the whole complex plane is made to simplify notation in some of the results. In fact one could compute a finite radius $R > 0$ such that analyticity in the disc $B_R(0)$ of radius R centred about the origin would suffice.

Given such a test function h the following trace is studied

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(\mathbf{1}_{\Lambda_L}\operatorname{Op}(\psi^{(b)}\mathcal{D})\mathbf{1}_{\Lambda_L}\big)\big], \qquad (2.50)$$

where $\Lambda := [0,2]^d \subset \mathbb{R}^d$ is the cube of side-length 2 and for a given scaling parameter $L > 0$, $\Lambda_L := [0,2L]^d$ is a scaled version of this cube. As Λ is bounded and $\psi^{(b)}$ is compactly supported, the operator in (2.50) is trace class, cf. again [BS87, Chap. 11, Sect. 8, Thm. 11]. For the trace (2.50), we obtain a multi-term asymptotic expansion in the scaling parameter L. We start by defining the coefficients occurring in the higher-order terms of this expansion. Using the abbreviation $X_{m,k,b} := \mathbf{1}_{\mathbb{R}_+^{m-k}\times\mathbb{R}^{d-m+k}}\operatorname{Op}(\psi^{(b)}\mathcal{D})\mathbf{1}_{\mathbb{R}_+^{m-k}\times\mathbb{R}^{d-m+k}}$ with $\mathbb{R}_+ := [0,\infty[$, we define

$$A_{m,h,b} := \lim_{L\to\infty}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\sum_{k=0}^{m} c_{k,m}\mathbf{1}_{[0,L]^m\times[0,1]^{d-m}}h\big(X_{m,k,b}\big)\Big], \qquad (2.51)$$

for $m \in \{0, \ldots, d-1\}$. The constants $c_{k,m}$ are given by $c_{k,m} := \frac{(-1)^k 2^m d!}{k!(m-k)!(d-m)!}$ for $0 \leqslant k \leqslant m \leqslant d-1$. We will see in Chapter 6 that these coefficients are well-defined. We note that the limits of the individual operators in the trace in (6.2) are not trace class and therefore the limit can not be interchanged with the trace. We further note that the index $m \in \{0, \ldots, d-1\}$ is not to be confused with the physical mass introduced in Section 2.2 which is always assumed to be zero in the present section.

For entire test functions h, we obtain a d-term asymptotic expansion and show that the remaining term is of order $\log L$.

Theorem 2.12. *Let $h : \mathbb{C} \to \mathbb{C}$ be an entire function satisfying $h(0) = 0$. Let $b \in [0, \infty[$, then the following asymptotic formula holds*

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[h\big(\mathbf{1}_{\Lambda_L}\operatorname{Op}(\psi^{(b)}\mathcal{D})\mathbf{1}_{\Lambda_L}\big)\right] = \sum_{m=0}^{d-1}(2L)^{d-m}A_{m,h,b} + O(\log L), \tag{2.52}$$

as $L \to \infty$. The coefficients $A_{m,h,b}$ are defined in (2.51). *The implied constant in the error term of order* $\log L$ *is independent of the ultraviolet cut-off parameter b.*

When the test function h is a polynomial of degree less or equal than three, we are able to compute the asymptotic coefficient of the subsequent logarithmic term and obtain the following $d+1$ term asymptotic expansion.

Theorem 2.13. *Let h be a polynomial of degree less or equal than three satisfying $h(0) = 0$. Let $b \in [0, \infty[$, then the following asymptotic formula holds*

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[h\big(\mathbf{1}_{\Lambda_L}\operatorname{Op}(\psi^{(b)}\mathcal{D})\mathbf{1}_{\Lambda_L}\big)\right] = {}&\sum_{m=0}^{d-1}(2L)^{d-m}A_{m,h,b}\\ &+ 2^d\,\log L\int_{S_+^{d-1}}\operatorname{tr}_{\mathbb{C}^n}[K_h(y,y)]\,\mathrm{d}y + O(1),\end{aligned} \tag{2.53}$$

as $L \to \infty$. Here, $S_+^{d-1} := \{y \in]0,\infty[^d : |y| = 1\} \subset S^{d-1}$ is the part of the unit sphere S^{d-1} which lies in the positive d-dimensional quadrant, and $K_h(y,y)$, $y \in S_+^{d-1}$ are the well-defined point-wise values of the continuous integral kernel K_h of the operator $\operatorname{Op}(\mathcal{D})_h$, *which is given by*

$$\operatorname{Op}(\mathcal{D})_h := \sum_{k=0}^{d}(-1)^k\sum_{\mathcal{M}\subseteq\{1,\ldots,d\}\,:\,|\mathcal{M}|=k} h(\mathbf{1}_{H_{\mathcal{M}}}\operatorname{Op}(\mathcal{D})\mathbf{1}_{H_{\mathcal{M}}}), \tag{2.54}$$

with $H_{\mathcal{M}} := \{x \in \mathbb{R}^d : \forall j \in \{1,\ldots,d\}\setminus\mathcal{M} : x_j \geqslant 0\}$.

The coefficients $A_{m,h,b}$, $m \in \{0,\ldots,d-1\}$, of the d leading terms of the asymptotic expansion, all depend on the ultraviolet cut-off parameter b. The coefficient of the logarithmic term is independent of b.

CHAPTER 3

Estimates for pseudo-differential operators with matrix-valued symbols

Context: In this preparatory chapter we present several estimates for pseudo-differential operators with matrix-valued symbols which will be needed in Chapters 4 and 5. The results and proofs, contained in the Sections 3.1 - 3.3, coincide to a large degree with the respective content from [BM24] and [BM25], both of which were written in collaboration with Peter Müller. The presentation of some of these results and proofs has been adapted to better fit the overall organisation of the present thesis. Some of the proofs have been extended.

Content: In the first section we collect estimates for the operator, trace-class and Schatten–von Neumann class norms of pseudo-differential operators with smooth, matrix-valued symbols. The estimates are straightforward extensions to matrix-valued symbols of the corresponding estimates for scalar-valued symbols which can be found in [Sob13] and [Sob14].

In the second section we consider Schatten–von Neumann class bounds for the commutator of an operator with smooth symbol and the projection onto an admissible domain. While the corresponding estimate is also a generalisation of an appropriate estimate in [Sob14], we not only extend it to the matrix-valued case but also require less strict assumptions on the admissible domain. These less strict requirements are helpful in the analysis carried out in Chapter 4.

In the third section we consider commutators as in section 3.2, but now with discontinuous matrix-valued symbols. The first estimate concerns symbols which are discontinuous at the boundary of an admissible domain and is, in the same sense as the estimate in Section 3.2, an extension of a corresponding result in [Sob14]. For the second estimate we consider symbols which are discontinuous at the origin. Here, we also prove the estimate in the scalar case. The proof also relies on the techniques used in [Sob14] and is similar to the proof of the estimate [FLS24, Lemma 4.3], which has recently been obtained independently of the estimate contained in this chapter.

Notation: In the proofs contained in this chapter we use the letters $C, C_1, C_2, C_{\nu\mu}$, etc. to denote generic positive constants whose value may differ from line to line.

3.1. Estimates for pseudo-differential operators with smooth symbols

We first give a proof that the matrix-valued operators (2.19) – (2.21) are bounded operators on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$ with operator norms $\|\cdot\|$ uniformly bounded in L. This is a simple reduction to the scalar case, which is contained in [Sob13, Chap. 3].

Lemma 3.1. *Let $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be a matrix-valued amplitude. Then for every $L \geqslant 1$ we have*

$$\|\operatorname{Op}_L^{lr}(A)\| \leqslant C\mathbf{N}^{(m,m,d+1)}(A) < \infty, \tag{3.1}$$

where $m := \lfloor \frac{d}{2} \rfloor + 1$, and the constant C is independent of L and A. Here, $\lfloor u \rfloor$ stands for the largest integer not exceeding $u \in \mathbb{R}$. Clearly, this carries over to symbols $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ so that

$$\| \operatorname{Op}_L^t(A)\| \leqslant C\mathbf{N}^{(m,d+1)}(A) < \infty \tag{3.2}$$

for both $t \in \{l, r\}$.

Proof. We use (2.27) and linearity to write

$$\| \operatorname{Op}_L^{lr}(A)\| = \Big\| \sum_{\nu,\mu=1}^{n} \operatorname{Op}_L^{lr}\big((A)_{\nu\mu}\big) \otimes E_{\nu\mu} \Big\| \leqslant \sum_{\nu,\mu=1}^{n} \big\| \operatorname{Op}_L^{lr}\big((A)_{\nu\mu}\big)\big\|. \tag{3.3}$$

By [Sob13, Lemma 3.9] we estimate, for every $\nu, \mu \in \{1, \dots, n\}$, that

$$\big\| \operatorname{Op}_L^{lr}\big((A)_{\nu\mu}\big)\big\| \leqslant C\mathbf{N}^{(m,m,d+1)}\big((A)_{\nu\mu}\big), \tag{3.4}$$

in terms of the symbol norm (2.23) for $n = 1$ and $s = \tau = 1$. This concludes the proof of the Lemma. □

We continue with bounds for pseudo-differential operators with smooth symbols which are compactly supported in both variables. But before we do so, we first give a definition of the Schatten–von Neumann classes.

Definition 3.2. Let $\mathcal{H}$ be a separable Hilbert space. For $q \in]0, \infty[$, we define the *Schatten–von Neumann class $\mathcal{T}_q$* as the vector space of all compact (linear) operators X on $\mathcal{H}$ with singular values $s_k(X) \in [0, \infty[$, $k \in \mathbb{N}$, such that

$$\|X\|_q := \Big(\sum_{k=1}^{\infty} s_k(X)^q \Big)^{\frac{1}{q}} < \infty. \tag{3.5}$$

Definition (3.5) induces a norm on $\mathcal{T}_q$ for $q \in [1, \infty[$. For $q \in]0, 1[$ it induces a quasi-norm for which the q-triangle inequality

$$\|X + Y\|_q^q \leqslant \|X\|_q^q + \|Y\|_q^q \tag{3.6}$$

holds for all $X, Y \in \mathcal{T}_q$. Furthermore, for every $q \in]0, \infty[$, a variant of Hölder's inequality holds, i.e. for $y \in \mathcal{T}_q$ and X a bounded linear operator on $\mathcal{H}$ we have

$$\|XY\|_q \leqslant \|X\|\|Y\|_q. \tag{3.7}$$

The following estimate is a straightforward generalisation of the scalar case in [Sob14, Thm 3.1].

Lemma 3.3. *Let $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be a matrix-valued symbol, whose support fulfils*

$$\operatorname{supp} A \subseteq B_s(u) \times B_\tau(v), \tag{3.8}$$

for some centres $u, v \in \mathbb{R}^d$ and radii $s, \tau > 0$ such that $s \geqslant 1$ and $L\tau \geqslant 1$. Then, for $t \in \{l, r\}$, we have

$$\| \operatorname{Op}_L^t(A)\|_q^q \leqslant C(Ls\tau)^d \big(\mathbf{N}^{(m_q,m_q)}(A; s, \tau)\big)^q, \tag{3.9}$$

where $m_q := \lfloor \frac{d}{q} \rfloor + 1$ and the constant C is independent of L, s, τ and A.

Proof. We reduce (3.30) to the scalar-valued case. We use (2.27) and the triangle inequality, to obtain

$$\| \operatorname{Op}_L^t(A)\|_q^q \leqslant \sum_{\nu,\mu=1}^{n} \big\| \operatorname{Op}_L^t\big((A)_{\nu\mu}\big) \otimes E_{\nu\mu}\big\|_q^q. \tag{3.10}$$

We now show that each individual term factorises in the tensor product. To see this, let $X \in \mathcal{T}_q$ be an operator on $L^2(\mathbb{R}^d)$ in the Schatten–von Neumann class corresponding to q and $M \in \mathbb{C}^{n\times n}$ be a matrix. We note that $|X \otimes M|^q = |X|^q \otimes |M|^q$. For rational number q, this is easy to verify. The equality extends to all $q \in]0,1]$ via the functional calculus. With this, we have

$$\|X \otimes M\|_q^q = \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[|X|^q \otimes |M|^q\right] = \left(\operatorname{tr}_{L^2(\mathbb{R}^d)}\left[|X|^q\right]\right)\left(\operatorname{tr}_{\mathbb{C}^n}\left[|M|^q\right]\right) = \|X\|_q^q \|M\|_q^q. \quad (3.11)$$

We warn the reader that the above equation involves three different Schatten–von Neumann-q-norms, on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$, on $L^2(\mathbb{R}^d)$ and on $\mathbb{C}^n$ from left to right. Using (3.11), we see that

$$\|\operatorname{Op}_L^t(A)\|_q^q \leqslant \sum_{\nu,\mu=1}^n \left\|\operatorname{Op}_L^t\left((A)_{\nu\mu}\right)\right\|_q^q, \quad (3.12)$$

which is the scalar case. An application of [Sob14, Thm. 3.1], yields

$$\left\|\operatorname{Op}_L^t\left((A)_{\nu\mu}\right)\right\|_q^q \leqslant C(Ls\tau)^d \left(\mathbf{N}^{(m_q,m_q)}(A;s,\tau)\right)^q, \quad (3.13)$$

for every $\nu,\mu \in \{1,\dots,n\}$. Defining $C := \sum_{\nu,\mu=1}^n C_{\nu\mu}$ concludes the proof of the Lemma, as $|M_{\nu\mu}| \leqslant \operatorname{tr}|M|$ for every matrix element $M_{\nu\mu}$ of a matrix M. □

Of particular importance for the proofs in Chapter 4, are operators, which are similar in the sense that a suitable Schatten–von Neumann norm of their difference is only of order L^{d-1} in the scaling parameter L. As we use this quite frequently, we introduce the following notation.

Definition 3.4. For $q \in]0,1]$ we write $X_L \sim_q Y_L$ for two L-dependent operators $X_L, Y_L \in \mathcal{T}_q$ of the corresponding Schatten–von Neumann class $\mathcal{T}_q$ over $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$, if there exists $C > 0$ such that $\|X_L - Y_L\|_q^q \leqslant CL^{d-1}$ for all $L \geqslant 1$. We further write $\sim$ for $\sim_1$.

In the special case of the trace norm, i.e. $q = 1$, there are several useful estimates in [Sob13, Chap. 3] which relate the left and the right operator quantisation and deal with products of operators. We also generalise these estimates to the matrix-valued case in the following Lemma. We emphasize that these estimates only hold for the trace norm and not general Schatten–von Neumann norms for $q \in]0,1[$, cf. [Sob14, Thm. 3.1].

Lemma 3.5. *Let $A, B \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be matrix-valued symbols and $F \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be a matrix-valued amplitude. We assume that B has compact support in both variables and F is compactly supported in ξ and in at least one of the variables x or y. We write D for the symbol given by $D(x,\xi) := F(x,x,\xi)$, for $x,\xi \in \mathbb{R}^d$. Then, for $t \in \{l,r\}$, we have*

$$\operatorname{Op}_L^l(B) \sim \operatorname{Op}_L^r(B) \quad (3.14)$$

and

$$\operatorname{Op}_L^{lr}(F) \sim \operatorname{Op}_L^l(D). \quad (3.15)$$

Further, we have

$$\operatorname{Op}_L^t(A)\operatorname{Op}_L^t(B) \sim \operatorname{Op}_L^t(AB) \quad (3.16)$$

and

$$\operatorname{Op}_L^t(B)\operatorname{Op}_L^t(A) \sim \operatorname{Op}_L^t(BA). \quad (3.17)$$

In the proof of Lemma 3.5 we provide more information on the constants arising in (3.14) – (3.17), see (3.22), (3.21), (3.28) and (3.29).

Proof. Let $L \geqslant 1$. In order to reduce (3.15) to the scalar-valued case, we use (2.27) and (3.11). The estimates in the scalar case can be found in [Sob13, Lemma 3.12]. Now assume that the support of the amplitude F fulfils

$$\operatorname{supp} F \subseteq B_s(u) \times \mathbb{R}^d \times B_\tau(v), \tag{3.18}$$

respectively

$$\operatorname{supp} F \subseteq \mathbb{R}^d \times B_s(u) \times B_\tau(v), \tag{3.19}$$

for $s, \tau > 0$ such that $Ls\tau \geqslant 1$. Then Lemma [Sob13, Lemma 3.12] even provides the bound

$$\left\| \operatorname{Op}_L^{lr}\left((F)_{\nu\mu}\right) - \operatorname{Op}_L^l\left((D)_{\nu\mu}\right)\right\|_1 \leqslant C(Ls\tau)^{d-1}\mathbf{N}^{(d+1,d+1,d+2)}\left((F)_{\nu\mu}; s, \tau\right), \tag{3.20}$$

for every $\nu, \mu \in \{1, \dots, n\}$, where the constant $C > 0$ is independent of L, s, τ and the amplitude F. Therefore, we obtain

$$\| \operatorname{Op}_L^{lr}(F) - \operatorname{Op}_L^l(D)\|_1 \leqslant C(Ls\tau)^{d-1}\mathbf{N}^{(d+1,d+1,d+2)}(F; s, \tau) \tag{3.21}$$

in terms of the norm (2.23) for matrix-valued amplitudes. The (new) constant $C > 0$ is independent of L, s, τ and the amplitude F. In the special case $F(x, y, \xi) = B(y, \xi)$, we obtain

$$\| \operatorname{Op}_L^r(B) - \operatorname{Op}_L^l(B)\|_1 \leqslant C(Ls\tau)^{d-1}\mathbf{N}^{(d+1,d+2)}(B; s, \tau), \tag{3.22}$$

which proves (3.14).

For (3.16) we use (2.27) to write

$$\begin{aligned} \operatorname{Op}_L^t(A)\operatorname{Op}_L^t(B) &= \left(\sum_{\nu,\mu=1}^n \operatorname{Op}_L^t\left((A)_{\nu\mu}\right) \otimes E_{\nu\mu}\right)\left(\sum_{\sigma,\kappa=1}^n \operatorname{Op}_L^t\left((B)_{\sigma\kappa}\right) \otimes E_{\sigma\kappa}\right) \\ &= \sum_{\nu,\mu,\kappa=1}^n \left(\operatorname{Op}_L^t\left((A)_{\nu\mu}\right)\operatorname{Op}_L^t\left((B)_{\mu\kappa}\right)\right) \otimes E_{\nu\kappa} \end{aligned} \tag{3.23}$$

and

$$\operatorname{Op}_L^t(AB) = \sum_{\nu,\kappa=1}^n \operatorname{Op}_L^t\left((AB)_{\nu\kappa}\right) \otimes E_{\nu\kappa} = \sum_{\nu,\mu,\kappa=1}^n \operatorname{Op}_L^t\left((A)_{\nu\mu}(B)_{\mu\kappa}\right) \otimes E_{\nu\kappa}. \tag{3.24}$$

Combining these two equalities, the triangle inequality and (3.11) yields

$$\left\| \operatorname{Op}_L^t(A)\operatorname{Op}_L^t(B) - \operatorname{Op}_L^t(AB)\right\|_1 \leqslant \sum_{\nu,\mu,\kappa=1}^n \left\| \operatorname{Op}_L^t\left((A)_{\nu\mu}\right)\operatorname{Op}_L^t\left((B)_{\mu\kappa}\right) - \operatorname{Op}_L^t\left((A)_{\nu\mu}(B)_{\mu\kappa}\right)\right\|_1. \tag{3.25}$$

The corresponding scalar estimates for $t = l$ are contained in [Sob13, Cor. 3.13]. The estimates for $t = r$ follow from taking the adjoint. If we assume that the support of the symbol B fulfils

$$\operatorname{supp} B \subseteq B_s(u) \times B_\tau(v), \tag{3.26}$$

for $s, \tau > 0$ such that $Ls\tau \geqslant 1$, [Sob13, Cor. 3.13] yields the more precise estimate

$$\begin{aligned} &\left\| \operatorname{Op}_L^t\left((A)_{\nu\mu}\right)\operatorname{Op}_L^t((B)_{\mu\kappa}) - \operatorname{Op}_L^t\left((A)_{\nu\mu}(B)_{\mu\kappa}\right)\right\|_1 \\ &\qquad \leqslant C(Ls\tau)^{d-1}\mathbf{N}^{(d+1,d+2)}\left((A)_{\nu\mu}; s, \tau\right)\mathbf{N}^{(d+1,d+2)}\left((B)_{\mu\kappa}; s, \tau\right) \end{aligned} \tag{3.27}$$

for every $\nu, \mu, \kappa \in \{1, \dots, n\}$, where the constant $C > 0$ is independent of L, s, τ and the symbols A, B. Therefore,

$$\left\| \operatorname{Op}_L^t(A)\operatorname{Op}_L^t(B) - \operatorname{Op}_L^t(AB)\right\|_1 \leqslant C(Ls\tau)^{d-1}\mathbf{N}^{(d+1,d+2)}(A; s, \tau)\,\mathbf{N}^{(d+1,d+2)}(B; s, \tau), \tag{3.28}$$

where the constant $C > 0$ is again independent of L, s, τ and the symbols A, B. This proves (3.16). The proof of (3.17) is analogous and yields

$$\left\| \operatorname{Op}_L^t(B)\operatorname{Op}_L^t(A) - \operatorname{Op}_L^t(BA)\right\|_1 \leqslant C(Ls\tau)^{d-1}\mathbf{N}^{(d+1,d+2)}(A; s, \tau)\,\mathbf{N}^{(d+1,d+2)}(B; s, \tau), \tag{3.29}$$

with the constant $C > 0$ again being independent of L, s, τ and the symbols A, B. This concludes the proof of the lemma. $\square$

3.2. Commutator estimates for smooth symbols

We now estimate the commutator of the left, respectively right, operator of a smooth, compactly supported symbol and a projection onto an admissible domain. We consider both the projections $\mathbf{1}_\Lambda$ and $\mathrm{Op}_L(\mathbf{1}_\Gamma)$ for admissible domains Λ, Γ. The estimates will be needed in the Schatten–von Neumann norm, for arbitrary $q \in]0,1]$, in both Chapters 4 and 5. In the scalar case with a symbol a being compactly supported in both variables and both Λ and Γ being bounded admissible domains or basic domains, the desired estimates were already established in [Sob14]. We extend these estimates to matrix-valued symbols A and to general (potentially unbounded) admissible domains Λ and Γ. While the extension to matrix-valued symbols is quite straightforward and similar to the proofs in Section 3.1, the extension to unbounded domains takes more effort. However, it is useful to obtain less strict requirements in the main results of Chapter 4, see Remark 4.30. As we will most often use the estimate in terms of the relation $\sim_q$, we state it in this form in Lemma 3.6. The disadvantage is that this notation does not track the dependence of the estimate on the size of the support of the matrix-valued symbol. Therefore, we also give a more detailed version of the estimate in Remark 3.7, which is necessary for one of the estimates in Section 3.3. The proof of Remark 3.7 is contained in the proof of Lemma 3.6.

Lemma 3.6. *Let $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be a matrix-valued symbol with compact support in both variables. Let Λ and Γ be admissible domains. Then, for every $q \in]0,1]$ and $t \in \{l, r\}$, the commutators obey*

$$\big[\mathrm{Op}_L^t(A), \mathbf{1}_\Lambda\big] \sim_q 0 \tag{3.30}$$

and

$$\big[\mathrm{Op}_L^t(A), \mathrm{Op}_L(\mathbf{1}_\Gamma)\big] \sim_q 0. \tag{3.31}$$

Remark 3.7. Suppose that in addition to the requirements in Lemma 3.6 one has

$$\operatorname{supp} A \subseteq B_s(u) \times B_\tau(v) \tag{3.32}$$

for some centres $u, v \in \mathbb{R}^d$ and radii $s, \tau > 0$ such that $s \geqslant 1$ and $L\tau \geqslant 1$. Then in the scalar-valued case Thm. 4.2 and Rem. 4.3 in [Sob14] provide a more precise estimate for the commutators in Lemma 3.6 depending on the radii s and τ of the support of the symbol A. As the proof of Lemma 3.6 will show this estimate extends to the matrix-valued case considered in Lemma 3.6 in the following way: Let $m_x := \lfloor \frac{d}{q} \rfloor + 1$ and $m_\xi := \lfloor \frac{d+1}{q} \rfloor + 1$. Then there exists a constant C which only depends on q and Λ such that

$$\big\|[\mathrm{Op}_L^t(A), 1_\Lambda]\big\|_q^q \leqslant C(Ls\tau)^{d-1}\big(\mathbf{N}^{(m_x, m_\xi)}(A; s, \tau)\big)^q, \tag{3.33}$$

where $\mathbf{N}^{(m_x, m_\xi)}(A; s, \tau)$ is defined in Definition 2.8.

Proof of Lemma 3.6. Let $L \geqslant 1$. We first want to reduce (3.30) to the scalar-valued case. We use (2.27) and estimate

$$\big\|\big[\mathrm{Op}_L^t(A), \mathbf{1}_\Lambda\big]\big\|_q^q \leqslant \sum_{\nu,\mu=1}^{n} \big\|\big[\mathrm{Op}_L^t\big((A)_{\nu\mu}\big), 1_\Lambda\big] \otimes E_{\nu\mu}\big\|_q^q. \tag{3.34}$$

With (3.11), we see that the individual terms on the right-hand side of (3.34) reduce to

$$\big\|\big[\operatorname{Op}_L^t\big((A)_{\nu\mu}\big), 1_\Lambda\big]\big\|_q^q, \tag{3.35}$$

which is the scalar case.

If Λ is a basic domain, Thm. 4.2 and Rem. 4.3 in [Sob14] yield constants $C_{\nu\mu}$, which only depend on q and Λ, such that

$$\big\|[\operatorname{Op}_L^t((A)_{\nu\mu}), 1_\Lambda]\big\|_q^q \leqslant C_{\nu\mu}(Ls\tau)^{d-1}\big(\mathbf{N}^{(m_x,m_\xi)}(A;s,\tau)\big)^q \tag{3.36}$$

for all $\nu,\mu \in \{1,\dots,n\}$. Here we used that $|M_{\nu\mu}| \leqslant \operatorname{tr}|M|$ for every matrix element $M_{\nu\mu}$ of a matrix M. Hence,

$$\big\|\big[\operatorname{Op}_L^t(A), \mathbf{1}_\Lambda\big]\big\|_q^q \leqslant C(Ls\tau)^{d-1}\big(\mathbf{N}^{(m_x,m_\xi)}(A;s,\tau)\big)^q, \tag{3.37}$$

where $C := \sum_{\nu,\mu=1}^n C_{\nu\mu}$ only depends on q and Λ. Therefore, it remains to show that the scalar result (3.36) extends to arbitrary admissible domains Λ. It suffices to show

$$\big\|1_\Lambda \operatorname{Op}_L^t(a)(1-1_\Lambda)\big\|_q^q \leqslant C(Ls\tau)^{d-1}\big(\mathbf{N}^{(m_x,m_\xi)}(a;s,\tau)\big)^q, \tag{3.38}$$

for an arbitrary scalar symbol $a \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ with compact support in both variables, as the estimate for the commutator follows from (3.38) together with its adjoint and the fact that (3.38) holds for both the left and the right operator.

In order to prove (3.38), define $\widetilde{\Lambda} := \{x \in \mathbb{R}^d : \operatorname{dist}(x,\Lambda) < s\}$ and let $R > 0$ such that the support of a in the first (i.e. space) variable is contained in $B_R(0)$. As Λ is admissible and $\overline{\widetilde{\Lambda} \cap B_R(0)}$ is compact, we can cover $\overline{\widetilde{\Lambda} \cap B_R(0)}$ with balls $B_\rho(x_j)$ with radius $\rho > 0$ and centres $x_j \in \mathbb{R}^d$, where $j \in \mathcal{J} \subset \mathbb{N}$ runs through some finite index set. The balls are chosen such that $\Lambda \cap B_{4\rho}(x_j) = \Lambda_j \cap B_{4\rho}(x_j)$ for every $j \in \mathcal{J}$, where Λ_j is a basic domain. We introduce a smooth partition of unity $\{\phi_j\}_{j\in\mathcal{J}}$ in $\mathbb{R}^d$ with $\operatorname{supp}\phi_j \subset B_\rho(x_j)$ for $j \in \mathcal{J}$ and

$$\Phi\big|_{\overline{\widetilde{\Lambda}\cap B_R(0)}} = 1, \qquad \text{where} \quad \Phi := \sum_{j\in\mathcal{J}} \phi_j \tag{3.39}$$

as well as

$$\sup_{x\in\mathbb{R}^d} |\partial_x^\alpha \phi_j(x)| \leqslant C\rho^{-|\alpha|}, \quad \alpha \in \mathbb{N}_0^d, \tag{3.40}$$

where the constant C does not depend on ρ. We start with the easier case $t = l$ and estimate

$$\big\|1_\Lambda \operatorname{Op}_L^l(a)(1-1_\Lambda)\big\|_q^q = \big\|1_\Lambda \Phi \operatorname{Op}_L^l(a)(1-1_\Lambda)\big\|_q^q \leqslant \sum_{j\in\mathcal{J}} \big\|1_{\Lambda_j}\phi_j \operatorname{Op}_L^l(a)(1-1_\Lambda)\big\|_q^q. \tag{3.41}$$

As the sum is finite, we just need to estimate the individual terms. We already have a basic domain to the left of the symbol. Therefore, it remains to also replace the occurrence of 1_Λ on the right-hand side by 1_{Λ_j} in order to complete the reduction.

For $j \in \mathcal{J}$, let $h_j \in C^\infty(\mathbb{R}^d)$ be a smooth function such that $\|h_j\|_\infty \leqslant 1$, $\operatorname{supp}(h_j) \subset B_{4\rho}(x_j)$ and $h_j|_{B_{2\rho}(x_j)} = 1$. We obtain

$$\begin{aligned}
\big\|1_{\Lambda_j}\phi_j \operatorname{Op}_L^l(a)(1-1_\Lambda)\big\|_q^q &= \big\|1_{\Lambda_j}\phi_j \operatorname{Op}_L^l(a)(h_j + 1 - h_j)(1-1_\Lambda)\big\|_q^q \\
&\leqslant \big\|1_{\Lambda_j}\phi_j \operatorname{Op}_L^l(a)h_j(1-1_{\Lambda_j})\big\|_q^q + \big\|\phi_j \operatorname{Op}_L^l(a)(1-h_j)\big\|_q^q \\
&\leqslant \big\|1_{\Lambda_j} \operatorname{Op}_L^l(\phi_j a)(1-1_{\Lambda_j})\big\|_q^q \\
&\quad + C(L\rho\tau)^{d-m_\xi q}\big(\mathbf{N}^{(m_x,m_\xi)}(\phi_j a;\rho,\tau)\big)^q,
\end{aligned} \tag{3.42}$$

with a constant C which only depends on q. Here, we used [Sob14, Thm. 3.2] with $\alpha = L$, $\ell_0 = \ell = R = \rho$, $h_1 = 1_{B_\rho(x_j)}$, $h_2 = 1 - h_j$ and $a = \phi_j a$ in the last step. This is possible, as the distance of the supports of ϕ_j and $1 - h_j$ is at least ρ by construction. Above, we used the notation $\mathrm{Op}_L^l(\phi_j a)$ which is abusive, as it does not specify the variable the function ϕ_j depends on. However, it should be still clear from the context and the definition of the function ϕ_j that the symbol $\phi_j a$ should be interpreted as $\phi_j a : \mathbb{R}^d \times \mathbb{R}^d \ni (x, \xi) \mapsto \phi_j(x) a(x, \xi)$.

As ρ only depends on Λ, the bound (3.40) allows us to estimate the second term in the last line of (3.42) from above by

$$C(L\tau)^{d - m_\xi q} \big(\mathbf{N}^{(m_x, m_\xi)}(a; 1, \tau)\big)^q \leqslant C(Ls\tau)^{d-1} \big(\mathbf{N}^{(m_x, m_\xi)}(a; s, \tau)\big)^q, \tag{3.43}$$

where the constant C now only depends on q and Λ and we used that $L\tau \geqslant 1$, $m_\xi q > d + 1 > 1$ as well as $s \geqslant 1$ in the last inequality. The estimates (3.41), (3.42) combined with (3.43) and (3.36) yield (3.38) for $t = l$.

For the more complicated case $t = r$, we write

$$\begin{aligned} \big\| 1_\Lambda \mathrm{Op}_L^r(a)(1 - 1_\Lambda) \big\|_q^q &= \big\| 1_\Lambda \mathrm{Op}_L^r(a)(\Phi + 1 - \Phi)(1 - 1_\Lambda) \big\|_q^q \\ &\leqslant \sum_{j \in \mathcal{J}} \big\| 1_\Lambda \mathrm{Op}_L^r(a)\phi_j(1 - 1_{\Lambda_j}) \big\|_q^q + \big\| 1_\Lambda \mathrm{Op}_L^r(a) 1_{B_R(0)}(1 - \Phi) \big\|_q^q. \end{aligned} \tag{3.44}$$

Note that $\mathrm{supp}(1 - \Phi) \subset \big(\overline{\widetilde{\Lambda} \cap B_R(0)}\big)^c \subset \widetilde{\Lambda}^c \cup \big(B_R(0)\big)^c$ and therefore $\mathrm{supp}\,\big(1_{B_R(0)}(1 - \Phi)\big) \subset \widetilde{\Lambda}^c$. Hence, the distance between the supports of 1_Λ and $1_{B_R(0)}(1 - \Phi)$ is at least s and [Sob14, Thm. 3.2] yields

$$\big\| 1_\Lambda \mathrm{Op}_L^r(a)(1 - 1_\Lambda) \big\|_q^q \leqslant \sum_{j \in \mathcal{J}} \big\| 1_\Lambda \mathrm{Op}_L^r(a)\phi_j(1 - 1_{\Lambda_j}) \big\|_q^q + C(Ls\tau)^{d - m_\xi q} \big(\mathbf{N}^{(m_x, m_\xi)}(a; s, \tau)\big)^q. \tag{3.45}$$

From here on, we continue similarly to the case of the left operator by inserting $h_j + (1 - h_j)$ to the left of $\mathrm{Op}_L^r(a)$. This yields (3.38) for $t = r$. Relation (3.31) follows in the same way by interchanging the roles of the variables x and ξ. □

3.3. Commutation estimates for discontinuous symbols

We continue with a q-norm estimate for symbols which are discontinuous at the $(d-1)$-dimensional boundary of an admissible domain $\Gamma \subset \mathbb{R}^d$. In the case that we additionally have a spatial restriction onto an admissible domain $\Lambda \subset \mathbb{R}^d$, the obtained bound is of order $L^{d-1} \log L$ in the scaling parameter L. The estimate will be crucial in order to close the asymptotics in Sections 4.4 - 4.6. The corresponding estimate for scalar-valued symbols is [Sob14, Cor. 4.7]. As in the case of the estimate in Lemma 3.6, we both extend the scalar estimate to matrix-valued symbols and to unbounded admissible domains.

Lemma 3.8. *Let $B \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n \times n})$ be a matrix-valued symbol with compact support in both variables. Let Λ and Γ be admissible domains. Then, for every $L \geqslant 2$, $t \in \{l, r\}$ and $q \in\,]0, 1]$, we have*

$$\big\| \mathbf{1}_\Lambda \mathrm{Op}_L(\mathbf{1}_\Gamma) \mathrm{Op}_L^t(B) \mathrm{Op}_L(\mathbf{1}_\Gamma) \mathbf{1}_{\Lambda^c} \big\|_q^q \leqslant C L^{d-1} \log L, \tag{3.46}$$

and

$$\big\| \mathrm{Op}_L(\mathbf{1}_\Gamma) \mathrm{Op}_L^t(B) \mathrm{Op}_L(\mathbf{1}_{\Gamma^c}) \big\|_q^q \leqslant C L^{d-1}. \tag{3.47}$$

The constants $C > 0$ are independent of the scaling parameter L.

Proof. We start by proving (3.46). By Lemma 3.6, we have

$$\mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Op}_L^t(B) \operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_{\Lambda^c} \sim_q \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Op}_L^t(B)\mathbf{1}_{\Lambda^c}. \tag{3.48}$$

By applying (3.11), we obtain

$$\begin{aligned}\left\|\mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Op}_L^t(B)\mathbf{1}_{\Lambda^c}\right\|_q^q &= \left\| \sum_{\nu,\mu=1}^n 1_\Lambda \operatorname{Op}_L(1_\Gamma) \operatorname{Op}_L^t\left((B)_{\nu\mu}\right)1_{\Lambda^c} \otimes E_{\nu\mu}\right\|_q^q \\ &\leqslant \sum_{\nu,\mu=1}^n \left\|1_\Lambda \operatorname{Op}_L(1_\Gamma) \operatorname{Op}_L^t\left((B)_{\nu\mu}\right)1_{\Lambda^c}\right\|_q^q. \end{aligned}\tag{3.49}$$

Therefore, it suffices to show

$$\|1_\Lambda \operatorname{Op}_L(1_\Gamma) \operatorname{Op}_L^t(b)1_{\Lambda^c}\|_q^q \leqslant CL^{d-1}\log L, \tag{3.50}$$

for an arbitrary scalar-valued symbol $b \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ with compact support in both variables. It follows, that there is some $R > 0$ such that the support of b is contained in $B_R(0) \times B_R(0)$.

As in the proof of Lemma 3.6, we define $\widetilde{\Lambda} := \{x \in \mathbb{R}^d : \operatorname{dist}(x, \Lambda) < R\}$ and cover $\overline{\widetilde{\Lambda} \cap B_R(0)}$ with balls $B_\rho(x_j)$ of radius ρ and centres x_j such that $\Lambda \cap B_{4\rho}(x_j) = \Lambda_j \cap B_{4\rho}(x_j)$, where Λ_j is a basic domain for every $j \in \mathcal{J} \subset \mathbb{N}$, with $\mathcal{J}$ being a finite index set. We also cover $\overline{\Gamma \cap B_R(0)}$ in the same manner with balls $B_{\rho_2}(\xi_k)$ of radius ρ_2 and centres ξ_k for $k \in \mathcal{K} \subset \mathbb{N}$, with $\mathcal{K}$ also being a finite index set. Let $\{\phi_j\}_{j\in\mathcal{J}}$, $\{\psi_k\}_{k\in\mathcal{K}}$ be smooth and finite partitions of unity subordinate to these coverings, i.e. we have $\operatorname{supp}\phi_j \subset B_\rho(x_j)$, $\operatorname{supp}\psi_k \subset B_{\rho_2}(\xi_k)$, as well as

$$\Phi\big|_{\overline{\widetilde{\Lambda}\cap B_R(0)}} = 1 \quad \text{and} \quad \Psi\big|_{\overline{\Gamma\cap B_R(0)}} = 1, \tag{3.51}$$

where $\Phi := \sum_{j\in\mathcal{J}} \phi_j$ and $\Psi := \sum_{k\in\mathcal{K}} \psi_k$. First, we treat the more difficult case $t = r$. We write

$$\begin{aligned}\left\|1_\Lambda \operatorname{Op}_L(1_\Gamma) \operatorname{Op}_L^r(b)1_{\Lambda^c}\right\|_q^q &= \left\|1_\Lambda \operatorname{Op}_L(1_\Gamma) \operatorname{Op}_L^r\left(b(\Phi + 1 - \Phi)\Psi\right)1_{\Lambda^c}\right\|_q^q \\ &\leqslant \left\|1_\Lambda \operatorname{Op}_L(1_\Gamma) \operatorname{Op}_L^r(b\Phi\Psi)1_{\Lambda^c}\right\|_q^q \\ &\quad + \left\|1_\Lambda \operatorname{Op}_L(1_\Gamma) \operatorname{Op}_L^r\left(b\left(1 - \Phi\right)\right)\right\|_q^q. \end{aligned}\tag{3.52}$$

As the symbol $b(1 - \Phi)$ is still smooth and compactly supported in both variables, we apply Lemma 3.6 to obtain

$$1_\Lambda \operatorname{Op}_L(1_\Gamma) \operatorname{Op}_L^r\left(b(1 - \Phi)\right) \sim_q 1_\Lambda \operatorname{Op}_L^r\left(b(1 - \Phi)\right) \operatorname{Op}_L(1_\Gamma). \tag{3.53}$$

We note that, as in the proof of Lemma 3.6, the support of $b(1 - \sum_j \phi_j)$ in the first variable is contained in $\widetilde{\Lambda}^c$ and therefore is of distance at least R to the support of the function 1_Λ. Therefore, we can apply [Sob14, Thm. 3.2] to obtain

$$\left\|1_\Lambda \operatorname{Op}_L^r\left(b(1 - \Phi)\right) \operatorname{Op}_L(1_\Gamma)\right\|_q^q \leqslant \left\|1_\Lambda \operatorname{Op}_L^r(b)(1 - \Phi)\right\|_q^q \leqslant C. \tag{3.54}$$

It remains to estimate

$$\left\|1_\Lambda \operatorname{Op}_L(1_\Gamma) \operatorname{Op}_L^r(b\Phi\Psi)1_{\Lambda^c}\right\|_q^q \leqslant \sum_{\substack{j\in\mathcal{J}\\ k\in\mathcal{K}}} \left\|1_\Lambda \operatorname{Op}_L(1_{\Gamma_k}) \operatorname{Op}_L^r(b\phi_j\psi_k)1_{\Lambda_j^c}\right\|_q^q. \tag{3.55}$$

As the sum is finite, it suffices to evaluate the individual terms. Using Lemma 3.6 again, we see that

$$1_\Lambda \operatorname{Op}_L(1_{\Gamma_k}) \operatorname{Op}_L^r(b\phi_j\psi_k)1_{\Lambda_j^c} \sim_q 1_\Lambda \operatorname{Op}_L^r(b\phi_j\psi_k) \operatorname{Op}_L(1_{\Gamma_k})1_{\Lambda_j^c}. \tag{3.56}$$

Let $h_j \in C^\infty(\mathbb{R}^d)$ be a smooth function such that $\|h_j\|_\infty \leqslant 1$, $\operatorname{supp}(h_j) \subset B_{4\rho}(x_j)$ and $h_j|_{B_{2\rho}(x_j)} = 1$. Then

$$\begin{aligned}\left\|1_\Lambda \operatorname{Op}_L^r(b\phi_j\psi_k)\operatorname{Op}_L(1_{\Gamma_k})1_{\Lambda_j^c}\right\|_q^q &= \left\|1_\Lambda(h_j + 1 - h_j)\operatorname{Op}_L^r(b\phi_j\psi_k)\operatorname{Op}_L(1_{\Gamma_k})1_{\Lambda_j^c}\right\|_q^q \\ &\leqslant \left\|1_{\Lambda_j}\operatorname{Op}_L^r(b\phi_j\psi_k)\operatorname{Op}_L(1_{\Gamma_k})1_{\Lambda_j^c}\right\|_q^q \\ &\quad + \|(1-h_j)\operatorname{Op}_L^r(b\psi_k)\phi_j\|_q^q. \end{aligned} \tag{3.57}$$

To obtain a bound for the last term we again apply [Sob14, Thm. 3.2], as the supports of $(1 - h_j)$ and ϕ_j have distance at least ρ. This yields

$$\|(1-h_j)\operatorname{Op}_L^r(b\psi_k)\phi_j\|_q^q \leqslant C. \tag{3.58}$$

In the remaining term all occurrences of admissible domains are replaced by basic domains and applying [Sob14, Thm. 4.6] yields

$$\left\|1_{\Lambda_j}\operatorname{Op}_L^r(b\phi_j\psi_k)\operatorname{Op}_L(1_{\Gamma_k})1_{\Lambda_j{}^c}\right\|_q^q \leqslant CL^{d-1}\log L. \tag{3.59}$$

Combining (3.52) – (3.59) yields (3.50) and concludes the proof of (3.46) for $t = r$. The simpler case $t = l$ starts from rewriting the operator in (3.50) as

$$1_\Lambda \operatorname{Op}_L(1_\Gamma)\operatorname{Op}_L^l(b)1_{\Lambda^c} \sim_q 1_\Lambda \operatorname{Op}_L^l(b)\operatorname{Op}_L(1_\Gamma)1_{\Lambda^c} = \sum_{\substack{j\in\mathcal{J}\\ k\in\mathcal{K}}} 1_{\Lambda_j}\phi_j \operatorname{Op}_L^l(b)\psi_k \operatorname{Op}_L(1_{\Gamma_k})1_{\Lambda^c}. \tag{3.60}$$

The further steps mirror the ones of the case $t = r$, starting from (3.56).

Finally, Inequality (3.47) is a direct consequence of Lemma 3.6. □

For the last bound presented in this chapter, we again consider commutators with projections onto admissible domains Λ. But now for operators with symbols which are discontinuous only at the origin and are smooth everywhere else. This is precisely the case for the free Dirac operator, if $E_F = m = 0$. As this is also our main motivation for this estimate, we only prove it for symbols which depend on a single variable ξ. Instead we focus on controlling the dependence of the bound on the size of the support of the symbol, as, in the application to the free Dirac operator, this quantifies the dependence on the chosen ultraviolet cut-off parameter.

As this type of discontinuity is somewhat specific to the Dirac operator, there is no scalar-valued version of this estimate in the previous literature that we could cite and extend directly. Instead we prove an additional Schatten–von Neumann estimate, also for scalar-valued symbols, whose proof is based upon the proof of [Sob14, Thm. 4.6]. A related estimate was recently obtained in [FLS24, Lemma 4.3]. Both estimates were obtained independently of one another.

Lemma 3.9. *Let Λ be a bounded admissible domain and $B \in C_b^\infty(\mathbb{R}^d \setminus \{0\}, \mathbb{C}^{n\times n})$ be a matrix-valued symbol which is discontinuous at the origin. Further assume that*

$$\operatorname{supp} B \subset B_{b+1}(0), \tag{3.61}$$

for a given parameter $b \geqslant 0$. Then there exists a constant $C > 0$, which is independent of L and b, such that for every $L \geqslant 2$ and $q \in]0,1]$

$$\left\|\mathbf{1}_\Lambda \operatorname{Op}_L(B)\mathbf{1}_{\Lambda^c}\right\|_q^q \leqslant C\begin{cases}\log[(b+1)L] & \text{if } d = 1,\\ [(b+1)L]^{d-1} & \text{if } d \geqslant 2.\end{cases} \tag{3.62}$$

Proof. Let $L \geqslant 2$ and define the function $\tau : \mathbb{R}^d \to \mathbb{R}_+$ by

$$\tau(\xi) := \frac{1}{4}\sqrt{\frac{1}{L^2} + |\xi|^2}. \tag{3.63}$$

It is clearly Lipschitz continuous on $\mathbb{R}^d$ with Lipschitz constant $\frac{1}{4}$. By [Hör03, Thm.1.4.10] this function gives rise to a sequence of centres $(\xi_j)_{j\in\mathbb{N}} \subset \mathbb{R}^d$ such that the balls of radius $\tau_j := \tau(\xi_j)$ about the points ξ_j cover $\mathbb{R}^d$, i.e. $\bigcup_{j\in\mathbb{N}} B_{\tau_j}(\xi_j) = \mathbb{R}^d$ and such that at most $N < \infty$ balls intersect in any given point, where the number N only depends on the dimension d. We refer to this last property as the finite-intersection property. Furthermore by [Hör03, Thm.1.4.10], there is a partition of unity $(\psi_j)_{j\in\mathbb{N}}$ subordinate to this covering, and for every multi-index $\alpha \in \mathbb{N}_0^d$ there exists a constant $\tilde{C}_{|\alpha|} > 0$ such that

$$\sup_{j\in\mathbb{N}} \sup_{\xi\in\mathbb{R}^d} |\partial_\xi^\alpha \psi_j(\xi)| \leqslant \tilde{C}_{|\alpha|} \tau(\xi)^{-|\alpha|}. \tag{3.64}$$

Here, $|\alpha| := \sum_{k=1}^d \alpha_k$. We note the (trivial) fact that $(\psi_j)_{j\in\mathbb{N}}$ is independent of b. The Lipschitz continuity of τ guarantees that for every $j \in \mathbb{N}$ and every $\xi \in B_{\tau_j}(\xi_j)$ the following inequality holds

$$\frac{4}{5}\tau(\xi) \leqslant \tau_j \leqslant \frac{4}{3}\tau(\xi). \tag{3.65}$$

As we have $\operatorname{supp} B \subset B_{b+1}(0)$, there is a finite index set $J \subset \mathbb{N}$, which depends on b, such that $\bigcup_{j\in J} B_{\tau_j}(\xi_j) \supseteq \operatorname{supp} B$. We divide J into two (finite) parts

$$J_1 := \{j \in J : B_{\tau_j}(\xi_j) \cap \{0\} \neq \varnothing\} \qquad \text{and} \qquad J_2 := J \setminus J_1. \tag{3.66}$$

The finite-intersection property implies the b-independent upper bound $|J_1| \leqslant N$. Using the q-triangle inequality, we estimate

$$\left\|\mathbf{1}_\Lambda \operatorname{Op}_L(B)\mathbf{1}_{\Lambda^c}\right\|_q^q \leqslant \sum_{j\in J_1} \left\|\mathbf{1}_\Lambda \operatorname{Op}_L(\psi_j B)\mathbf{1}_{\Lambda^c}\right\|_q^q + \sum_{j\in J_2} \left\|\mathbf{1}_\Lambda \operatorname{Op}_L(\psi_j B)\mathbf{1}_{\Lambda^c}\right\|_q^q. \tag{3.67}$$

If $j \in J_1$, we estimate

$$\left\|\mathbf{1}_\Lambda \operatorname{Op}_L(\psi_j B)\mathbf{1}_{\Lambda^c}\right\|_q^q \leqslant \left\|\operatorname{Op}_L^l\left(\phi\psi_j \otimes \mathbb{1}_n\right)\right\|_q^q \left\|\operatorname{Op}_L(B)\right\|^q, \tag{3.68}$$

where $\phi \in C_c^\infty(\mathbb{R}^d)$ with $\phi|_\Lambda = 1$ is supported in the ball $B_{r_1}(0)$ for some radius $r_1 > 0$. As the operator $\operatorname{Op}_L(B)$ has operator norm bounded independently of L and b, it remains to estimate the q-norm of the operator $\operatorname{Op}_L^l\left(\phi\psi_j \otimes \mathbb{1}_n\right)$. As $0 \in B_{\tau_j}(\xi_j)$ for all $j \in J_1$, property (3.65) guarantees that $\phi\psi_j$ is compactly supported in $B_{r_1}(0) \times B_{\frac{1}{3L}}(\xi_j)$. Therefore, by an application of Lemma 3.3 the right-hand side of (3.68) is bounded from above by a constant C_1, independently of L and b. This, in turn, provides the bound

$$\sum_{j\in J_1} \left\|\mathbf{1}_\Lambda \operatorname{Op}_L(\psi_j B)\mathbf{1}_{\Lambda^c}\right\|_q^q \leqslant NC_1, \tag{3.69}$$

where the right-hand side is independent of L and b.

If instead $j \in J_2$ we note that the symbol $\psi_j B$ is smooth with $\operatorname{supp}\psi_j B \subset B_{\tau_j}(\xi_j) \subset B_{4\tau_j}(\xi_j)$. Since $4L\tau_j \geqslant 1$, we can apply Remark 3.7 with $A = \phi\psi_j B$, $t = l$, $s = \max\{r_1, 1\}$ and $\tau = 4\tau_j$, in order to obtain

$$\begin{aligned}\left\|\mathbf{1}_\Lambda \operatorname{Op}_L(\psi_j B)\mathbf{1}_{\Lambda^c}\right\|_q^q &= \left\|\mathbf{1}_\Lambda \operatorname{Op}_L^l(\phi\psi_j B)\mathbf{1}_{\Lambda^c}\right\|_q^q \\ &\leqslant C_2(L\tau_j)^{d-1}\left(\mathbf{N}^{(m_x,m_\xi)}(\phi\psi_j B;\max\{r_1,1\},\tau_j)\right)^q,\end{aligned} \tag{3.70}$$

where the constant $C_2 > 0$ is independent of $j \in J_2$, as well as of L and b and m_x, m_ξ are defined in Remark 3.7. Using (3.64), we conclude that

$$\left\|\mathbf{1}_\Lambda \operatorname{Op}_L(\psi_j B)\mathbf{1}_{\Lambda^c}\right\|_q^q \leqslant C_3(L\tau_j)^{d-1}, \tag{3.71}$$

where the constant $C_3 > 0$ is again independent of $j \in J_2$, as well as of L and b. Therefore, we have

$$\sum_{j\in J_2} \left\|\mathbf{1}_\Lambda \operatorname{Op}_L\left(\psi_j B\right)\mathbf{1}_{\Lambda^c}\right\|_q^q \leqslant C_3 L^{d-1} \sum_{j\in J_2} \tau_j^{d-1}. \tag{3.72}$$

We now study the sum $\sum_{j\in J_2}\tau_j^{d-1}$ in more detail. Due to the bound (3.65) we see that

$$\tau_j^{d-1} = \frac{1}{|B_1(0)|}\int_{B_{\tau_j}(\xi_j)} \tau_j^{-1}\,\mathrm{d}\xi \leqslant \frac{4}{3|B_1(0)|}\int_{B_{\tau_j}(\xi_j)} \tau(\xi)^{-1}\,\mathrm{d}\xi, \tag{3.73}$$

for every $j \in J_2$. The definition (3.63) of τ, together with the definition of J and the compact support (3.61) of the symbol B, implies that the support $\operatorname{supp}\sum_{j\in J_2} 1_{B_{\tau_j}(\xi_j)}$ of the sum of all indicator functions of balls corresponding to the index set J_2 is contained in the ball $B_{2(b+1)}(0)$ of radius $2(b+1)$ about the origin. Therefore, the finite-intersection property yields the bound

$$\sum_{j\in J_2} 1_{B_{\tau_j}(\xi_j)}(\xi) \leqslant N 1_{B_{2(b+1)}(0)}(\xi), \tag{3.74}$$

for every $\xi \in \mathbb{R}^d$. Combining (3.73) and (3.74), we obtain the bound

$$C_3 L^{d-1}\sum_{j\in J_2}\tau_j^{d-1} \leqslant C_4 L^{d-1}\int_{\mathbb{R}^d}\sum_{j\in J_2} 1_{B_{\tau_j}(\xi_j)}(\xi)\tau(\xi)^{-1}\,\mathrm{d}\xi \leqslant C_4 N L^{d-1}\int_{B_{2(b+1)}(0)} \tau(\xi)^{-1}\mathrm{d}\xi, \tag{3.75}$$

where the constant $C_4 > 0$ is independent of L and b. Using the abbreviation $\rho := 2(b+1)$ and introducing spherical coordinates, the right-hand side of (3.75) reads

$$C_4 N|S^{d-1}|\int_0^{L\rho} \frac{r^{d-1}}{\sqrt{1+r^2}}\,\mathrm{d}r \leqslant C_5 \begin{cases} \log(\rho L) & \text{if } d = 1, \\ (\rho L)^{d-1} & \text{if } d \geqslant 2, \end{cases} \tag{3.76}$$

for some constant $C_5 > 0$ that is independent of L and b. Here, $|S^{d-1}|$ denotes the $(d-1)$-dimensional surface area of the unit sphere S^{d-1} induced by Lebesgue measure. This estimate, together with (3.75), (3.69) and (3.67) concludes the proof due to $(b+1)L \geqslant 2$. □

CHAPTER 4

The Widom–Sobolev formula for matrix-valued symbols

Context: The results contained in this chapter coincide with the results in [BM24] which was written in collaboration with Peter Müller. The contents of Section 4.1 partially agree with the beginning of [BM24] but have been extended. Large parts of the Sections 4.2 - 4.6 agree, in both content and writing, with the corresponding sections of [BM24]. Several of the proofs in these sections have been extended, and the presentation of the content has been adapted to better suit the larger context of the present thesis.

Content: In this chapter we consider general smooth bounded matrix-valued symbols. For these symbols we prove a Widom–Sobolev formula for several cases of test functions and different types of discontinuities in momentum space. We begin with polynomial test functions and a single cut-off region Γ in momentum space. We reduce this case to the local Widom–Sobolev formula in the scalar case, proved in [Sob13]. We then deal with more general types of discontinuities at the boundary of Γ by splitting $\mathbb{R}^d$ into Γ and its complement. The approach is based on the work in [Sob17]. It features additional challenges due to the presence of two, not necessarily commuting, matrix-valued symbols. Lastly, we extend the asymptotic expansion from polynomials to more general test functions. This "closing of the asymptotics" follows the strategies laid out in [Sob13, Sob17]. Again, the matrix nature of the symbols introduces some additional challenges.

Notation: In the proofs contained in this chapter we use the letters $C, C_1, C_2, C_{\nu\mu}$, etc. to denote generic positive constants whose value may differ from line to line.

4.1. Discussion of results and strategy of the proof

We use the notation introduced in Section 2.1. The goal of the present chapter is to prove several versions of the Widom–Sobolev formula for traces of test functions of operators with discontinuous matrix-valued symbols. We recall the definitions of the considered operators from Section 2.1:

$$D_L(A_1, A_2; \Lambda, \Gamma) = \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Op}_L^l(A_1) \operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda + \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \operatorname{Op}_L^l(A_2) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Lambda, \quad (4.1)$$

as well as its symmetrised version

$$\begin{aligned} G_L(A_1, A_2; \Lambda, \Gamma) = {} & \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Re}\big[\operatorname{Op}_L^l(\operatorname{Re} A_1)\big] \operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda \\ & + \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \operatorname{Re}\big[\operatorname{Op}_L^l(\operatorname{Re} A_2)\big] \operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Lambda. \end{aligned} \quad (4.2)$$

The three main results of this chapter are Theorem 4.14 for analytic test functions h, Theorem 4.22 for smooth test functions h and Theorem 4.29 for test functions h satisfying Assumption 2.5. We note that the last result, Theorem 4.29, includes all Rényi entropy functions, in particular the von Neumann entropy function, and is therefore of particular importance with regards to applications to the entanglement entropy.

As the test functions increase in generality, the allowed symbols decrease in generality. More precisely, if we study the operator $X_L(A_1, A_2; \Lambda, \Gamma)$ with $X \in \{D, G\}$, we require one of the following three assumptions to hold:

($\mathcal{A}1$) the function h is analytic in a disc of sufficiently large radius with $h(0) = 0$;
($\mathcal{A}2$) the function $h \in C^\infty(\mathbb{R})$ is smooth with $h(0) = 0$ and $X = G$;
($\mathcal{A}3$) the function satisfies Assumption 2.5 with $h(0) = 0$, we have $X = G$ and the symbols A_1 and A_2 only depend on the single variable ξ.

Operator sums as in (4.1) and (4.2) describe general jump discontinuities of the symbol at the boundary of Γ. While studying these sums is necessary for the application to the free Dirac operator in Chapter 5, it also constitutes an additional technical challenge in the case that the matrix-valued symbols A_1 and A_2 do not commute. Still, careful analysis in the proof of Theorem 4.5 allows us to obtain coefficients similar to the scalar-valued case. For scalar-valued symbols, such operator sums were already studied in [Sob17, Thm. 5.2]. In addition to working with matrix-valued symbols, we require slightly weaker assumptions on Γ and on the symbols A_1 and A_2, which is possible due to the fact that both Lemma 3.6 and Lemma 3.8 from the last chapter allow both Λ as well as Γ to be unbounded. This fact also simplifies several other steps in the proof of the main results. For Γ, A_1 and A_2 we require at least one of the following three assumptions to be fulfilled:

($\mathcal{B}1$) the domain Γ is bounded and A_2 is compactly supported in the second variable;
($\mathcal{B}2$) the domain Γ^c is bounded and A_1 is compactly supported in the second variable;
($\mathcal{B}3$) both the symbols A_1 and A_2 are compactly supported in the second variable.

The following theorem summarises the contents of Theorems 4.14, 4.22 and 4.29 in a slightly simplified version

Theorem 4.1. *Let $A_1, A_2 \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be matrix-valued symbols. Let Λ be a bounded piece-wise C^1-admissible domain and Γ be a piece-wise C^3-admissible domain. Let $X \in \{D, G\}$. If at least one of the assumptions ($\mathcal{A}1$)-($\mathcal{A}3$) is fulfilled and at least one of the assumptions ($\mathcal{B}1$)-($\mathcal{B}3$) is fulfilled, the following asymptotic formula holds*

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[h\big(X_L(A_1,A_2;\Lambda,\Gamma)\big)\right] = {} & L^d\Big(\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(A_1)];\Lambda,\Gamma\big)+\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(A_2)];\Lambda,\Gamma^c\big)\Big)\\ & + L^{d-1}\log L\ \mathfrak{W}_1\big(\mathfrak{U}(h;A_1,A_2);\partial\Lambda,\partial\Gamma\big)\\ & + o(L^{d-1}\log L),\end{aligned}\tag{4.3}$$

as $L \to \infty$. Here, the coefficients $\mathfrak{W}_0$ and $\mathfrak{W}_1$ were defined in (2.15) *and* (2.16)*, respectively, and the symbol $\mathfrak{U}$ in* (2.32)*.*

Both the coefficients $\mathfrak{W}_0$ and $\mathfrak{W}_1$ are scalar-valued, as the first argument of $\mathfrak{W}_0$ is a (scalar-valued) matrix trace and the symbol $\mathfrak{U}$, whose definition (2.32) we recall here

$$\mathfrak{U}(g;B_1,B_2) = \frac{1}{(2\pi)^2}\int_0^1 \frac{\operatorname{tr}_{\mathbb{C}^n}\left[g\big(B_1 t + B_2(1-t)\big) - g(B_1)t - g(B_2)(1-t)\right]}{t(1-t)}\,\mathrm{d}t, \tag{4.4}$$

is scalar-valued. We point out that the coefficients $\mathfrak{W}_0$ and $\mathfrak{W}_1$ are the same as in the scalar-valued case. In the one-dimensional case, this could already be seen in Widom [Wid82]. In fact, one could say that the coefficients in (4.3) are the simplest possible extensions of the scalar coefficients to the matrix case, just featuring an additional matrix trace. This is due to the fact that the matrix-structure can be reduced up to error terms of order L^{d-1}, as we will see in Section 4.2.

We note that the assumption that the symbols A_1 and A_2 are smooth is not strictly necessary and is made mostly for convenience. In fact, for analytic and smooth test functions, it would suffice to have finite symbol norms $\mathbf{N}^{(d+2,d+2)}(A_1)$ and $\mathbf{N}^{(d+2,d+2)}(A_2)$. For the definition of the symbol norm see Definition 2.8. In the case of the more general test functions, it would not suffice to consider the norm $\mathbf{N}^{(d+2,d+2)}$. One would need to have finite symbol norms $\mathbf{N}^{(n_\gamma,n_\gamma)}$ for a natural number $n_\gamma > \frac{d+1}{\gamma} + 1$ depending on the parameter γ from Assumption 2.5. The assumptions ($\mathcal{A}1$)-($\mathcal{A}3$) and ($\mathcal{B}1$)-($\mathcal{B}3$) are essential for the proof. In condition ($\mathcal{A}2$) the fact that $h \in C^\infty(\mathbb{R})$ is smooth is primarily used in Lemma 4.19 and could be slightly relaxed. A finite algebraic decay, depending on the dimension d, of the Fourier transform of h would suffice. The fact that A_1 and A_2 only depend on momentum space in ($\mathcal{A}3$) is crucial, as a version of Lemma 4.19 is not available for these more general test functions. The requirements for compact support in the assumptions ($\mathcal{B}1$)-($\mathcal{B}3$) can be replaced by the assumption that the appropriate symbol is Schwartz, cf. the assumptions in [Wid82].

We now give an overview of the strategy used to prove the main results of this chapter. For a given class of test functions, the proof can be subdivided into four steps. We first prove the Widom–Sobolev formula for polynomial test functions and a single matrix-valued symbol $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ which we cut off at the boundary of the domain Γ in momentum space, i.e. , for arbitrary $p \in \mathbb{N}$, we are interested in the trace

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\big(T_L(A)\big)^p\right] = \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\Big(\mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma)\operatorname{Op}_L^l(A)\operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda\Big)^p\right]. \tag{4.5}$$

Following the established strategies in [Wid82, Sob13, Sob15], this task consists of two steps. In the first of these steps we localise the problem and commute out the symbol A, up to an error term of order L^{d-1}, by utilising the estimates from Chapter 3. More precisely, suppose that the symbol A is compactly supported in both variables and localised in such a way that Λ is equal to some basic domain Λ_0 on the support of A and Γ is equal to some basic domain Γ_0 on the support of A. Then we show that

$$\Big(\mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma)\operatorname{Op}_L^l(A)\operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda\Big)^p \sim \operatorname{Op}_L^l(A^p)\big(\mathbf{1}_{\Lambda_0}\operatorname{Op}_L(\mathbf{1}_{\Gamma_0})\mathbf{1}_{\Lambda_0}\big)^p, \tag{4.6}$$

where we recall the definition of $\sim$ in Definition 3.4.

The second step is to provide a local asymptotic formula for the trace of the right-hand side of (4.6). Here, the reduction to the scalar-valued case happens. The key observation is that the commutation in the previous step already separated the matrix-structure of the symbol from the structure of the operator in the following sense. Interpreting $\operatorname{tr}_{\mathbb{C}^n}[A^p]$ as a smooth scalar-valued symbol, the factorisation of the trace in the tensor product yields the equality

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\operatorname{Op}_L^l(A^p)\big(\mathbf{1}_{\Lambda_0}\operatorname{Op}_L(\mathbf{1}_{\Gamma_0})\mathbf{1}_{\Lambda_0}\big)^p\right] = \operatorname{tr}_{L^2(\mathbb{R}^d)}\left[\operatorname{Op}_L^l(\operatorname{tr}_{\mathbb{C}^n}[A^p])\big(\mathbf{1}_{\Lambda_0}\operatorname{Op}_L(\mathbf{1}_{\Gamma_0})\mathbf{1}_{\Lambda_0}\big)^p\right]. \tag{4.7}$$

The trace on the right-hand side of (4.7) can be evaluated asymptotically with the local asymptotic formula in the scalar-valued case [Sob15, Thm. 4.1] in the case $d \geqslant 2$, respectively [Wid82] in the case $d = 1$. Both step one and two are carried out in Section 4.2 of this chapter.

In the third step, carried out in Section 4.3, we extend the asymptotic formula to the more general operator D_L. We recall that it is given by

$$D_L(A_1, A_2; \Lambda, \Gamma) = T_L(A_1; \Lambda, \Gamma) + T_L(A_2; \Lambda, \Gamma^c). \tag{4.8}$$

For scalar-valued symbols this operator has already been studied in [Sob17, Sec. 5] and we extend the corresponding proof. Up to an error of order L^{d-1} we rewrite the right-hand side of (4.8) as

$$T_L(A_2; \Lambda, \mathbb{R}^d) + T_L(A_1 - A_2; \Lambda, \Gamma). \tag{4.9}$$

In order to analyse the trace of a power of this operator, we evaluate each of the products, arising in the corresponding sum, individually, using the asymptotic formula obtained in the first two steps of our proof. As we do not require the symbols A_1 and A_2 to commute, the operators $T_L(A_2; \Lambda, \mathbb{R}^d)$

and $T_L(A_1 - A_2; \Lambda, \Gamma)$ might also not commute. Therefore, we need to take additional care when writing out

$$\big(T_L(A_2; \Lambda, \mathbb{R}^d) + T_L(A_1 - A_2; \Lambda, \Gamma)\big)^p \tag{4.10}$$

as a sum. Still, collecting all contributions to the trace, we exactly obtain the structure of the symbol $\mathfrak{U}$.

The fourth step is the extension from polynomials to the desired class of test functions. This closing of the asymptotics essentially follows the strategies laid out in [Sob13, Chap. 12] (for analytic and smooth test functions) and [Sob17, Sec. 4] (for the more general test functions). Most of the intermediate results need to be adapted to the situation at hand. In some cases this is quite straightforward, in other cases the matrix-valued symbols, combined with the structure of the operators D_L, G_L, lead to additional technical challenges. This last step is carried out in Sections 4.4 - 4.6 for the three different classes of test functions.

4.2. Asymptotic formula for polynomials

As outlined in the strategy of the proof we begin by proving the asymptotic expansion for polynomial test functions and the operator $T_L(A)$. By linearity this reduces to the case of monomial test functions. We are therefore faced with the task of calculating

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\big(T_L(A)\big)^p\right] = \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\Big(\mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma)\operatorname{Op}_L^l(A)\operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda\Big)^p\right] \tag{4.11}$$

for $p \in \mathbb{N}$. In order to reduce this to the scalar-valued case, we need to deal with the matrix structure. To do so, we commute the p occurrences of the operator $\operatorname{Op}_L^l(A)$ to the left up to area terms by using the estimates contained in Sections 3.1 and 3.2.

The first ingredient for the monomial case is the following lemma which applies the results from Chapter 3 to the situation at hand.

Lemma 4.2. *Let $A, B \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be matrix-valued symbols and assume that B is compactly supported in both variables. Let Λ and Γ be admissible domains. Further, let Λ_0 and Γ_0 be basic domains such that*

$$B\big|_{\Lambda\times\mathbb{R}^d} = B\big|_{\Lambda_0\times\mathbb{R}^d} \qquad \text{and} \quad B\big|_{\mathbb{R}^d\times\Gamma} = B\big|_{\mathbb{R}^d\times\Gamma_0}. \tag{4.12}$$

Then, for $p \in \mathbb{N}$, we have

$$\operatorname{Op}_L^l(B)\big(T_L(A; \Lambda, \Gamma)\big)^p \sim \operatorname{Op}_L^l(BA^p)\big(T_L(\mathbb{1}_n; \Lambda_0, \Gamma_0)\big)^p. \tag{4.13}$$

Proof. The symbol B is compactly supported in both variables. Therefore, we can apply Lemmas 3.5 and 3.6. By assumption we have $\mathbf{1}_\Lambda \operatorname{Op}_L^l(B) = \mathbf{1}_{\Lambda_0}\operatorname{Op}_L^l(B)$ and $\operatorname{Op}_L^l(B)\operatorname{Op}_L(\mathbf{1}_\Gamma) = \operatorname{Op}_L^l(B)\operatorname{Op}_L(\mathbf{1}_{\Gamma_0})$. Therefore, we obtain

$$\operatorname{Op}_L^l(B)\mathbf{1}_\Lambda \sim \mathbf{1}_\Lambda \operatorname{Op}_L^l(B) = \mathbf{1}_{\Lambda_0}\operatorname{Op}_L^l(B) \tag{4.14}$$

and

$$\operatorname{Op}_L^l(B)\operatorname{Op}_L(\mathbf{1}_\Gamma) = \operatorname{Op}_L^l(B)\operatorname{Op}_L(\mathbf{1}_{\Gamma_0}) \sim \operatorname{Op}_L(\mathbf{1}_{\Gamma_0})\operatorname{Op}_L^l(B). \tag{4.15}$$

Furthermore, an application of (3.16) yields

$$\operatorname{Op}_L^l(B)\operatorname{Op}_L^l(A) \sim \operatorname{Op}_L^l(BA). \tag{4.16}$$

We note that the three relations above still hold, if one replaces the symbol B by BA^m for some $m \in \mathbb{N}$. Repeatedly applying the relations, starting from the left, yields

$$\operatorname{Op}_L^l(B)\big(T_L(A; \Lambda, \Gamma)\big)^p \sim \big(T_L(\mathbb{1}_n; \Lambda_0, \Gamma_0)\big)^p \operatorname{Op}_L^l(BA^p). \tag{4.17}$$

The symbol BA^p is still compactly supported in both variables. Therefore, repeated application of Lemma 3.6 yields the desired result. □

The next crucial ingredient is the local asymptotic formula for basic domains. This is an extension to matrix-valued symbols of the appropriate scalar results, namely [Sob15, Thm. 4.1] in the case that $d \geqslant 2$ and the initial result by Widom [Wid82] in the case $d = 1$.

Theorem 4.3 (Local asymptotic formula)**.** *Let $p \in \mathbb{N}$, let Λ be a piece-wise C^1-basic domain and Γ be a piece-wise C^3-basic domain. Further let $B \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be a matrix-valued symbol with compact support in both variables. Then*

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\operatorname{Op}_L^l(B)\big(T_L(\mathbb{1}_n;\Lambda,\Gamma)\big)^p\Big] &= L^d\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[B];\Lambda,\Gamma\big)\\ &\quad + L^{d-1}\log L\ \mathfrak{W}_1\big(\operatorname{tr}_{\mathbb{C}^n}[B]\,\mathfrak{U}(g_p;1);\partial\Lambda,\partial\Gamma\big)\\ &\quad + o(L^{d-1}\log L), \end{aligned}\tag{4.18}$$

as $L \to \infty$. Here, g_p is the monomial of degree p, the coefficients $\mathfrak{W}_0$ and $\mathfrak{W}_1$ are defined in (2.15) *and* (2.16)*, respectively, and we refer to* (2.17) *for the definition of the symbol $\mathfrak{U}$.*

Proof. Writing out the symbol in form of a tensor product and using that $\operatorname{tr}_{\mathbb{C}^n}[E_{\nu\mu}] = \delta_{\nu,\mu}$, where $\delta_{\nu,\mu}$ is the Kronecker delta, we obtain

$$\begin{aligned}&\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\operatorname{Op}_L^l(B)\big(T_L(\mathbb{1}_n;\Lambda,\Gamma)\big)^p\Big]\\ &\qquad= \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Bigg[\sum_{\nu,\mu=1}^n \operatorname{Op}_L^l\big((B)_{\nu\mu}\otimes E_{\nu\mu}\big)\big(T_L(1)\otimes\mathbb{1}_n\big)^p\Bigg]\\ &\qquad= \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Bigg[\sum_{\nu,\mu=1}^n \operatorname{Op}_L^l\big((B)_{\nu\mu}\big)\big(T_L(1)\big)^p\otimes E_{\nu\mu}\Bigg]\\ &\qquad= \sum_{\nu=1}^n \operatorname{tr}_{L^2(\mathbb{R}^d)}\Big[\operatorname{Op}_L^l\big((B)_{\nu\nu}\big)\big(T_L(1)\big)^p\Big]\\ &\qquad= \operatorname{tr}_{L^2(\mathbb{R}^d)}\Big[\operatorname{Op}_L^l\big(\operatorname{tr}_{\mathbb{C}^n}[B]\big)\big(T_L(1)\big)^p\Big]. \end{aligned}\tag{4.19}$$

In the second to last step we used that the trace factorises for elementary tensor products. The scalar-valued symbol $\operatorname{tr}_{\mathbb{C}^n}[B] = \sum_{\nu=1}^n (B)_{\nu\nu}$ is clearly smooth as a sum of smooth scalar-valued symbols. The asymptotics for this last term is given by [Sob15, Thm. 4.1] in the case that $d \geqslant 2$:

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)}\big[\operatorname{Op}_L^l\big(\operatorname{tr}_{\mathbb{C}^n}[B]\big)\big(T_L(1)\big)^p\big] &= L^d\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[B];\Lambda,\Gamma\big)\\ &\quad + L^{d-1}\log L\ \mathfrak{W}_1\big(\operatorname{tr}_{\mathbb{C}^n}[B]\,\mathfrak{U}(g_p;1);\partial\Lambda,\partial\Gamma\big)\\ &\quad + o(L^{d-1}\log L), \end{aligned}\tag{4.20}$$

as $L \to \infty$.

For the case $d = 1$ we use the initial result by Widom [Wid82]. As translation, reflection and time reversal are unitary operators, we just need to consider the case $\Lambda = \Gamma =]0,\infty[$. Commuting $\operatorname{Op}_L^l(\operatorname{tr}_{\mathbb{C}^n}[B])$ to the right is possible up to area terms by Lemma 3.6. Taking $f = g_p$, we are now in the situation of [Wid82, Eq. (12)] up to multiplication with the constant $\operatorname{tr}_{\mathbb{C}^n}[B](0,0)$. The desired asymptotic formula follows. □

With these tools at hand, we are now ready to prove the asymptotic expansion for polynomials.

Theorem 4.4. *Let $p \in \mathbb{N}$, let $A, B \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be matrix-valued symbols. Let Λ be a bounded piece-wise C^1-admissible domain and Γ be a piece-wise C^3-admissible domain. We assume Γ to be bounded or one of the symbols A respectively B to be compactly supported in the second variable. Then*

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\operatorname{Op}_L^l(B)\big(T_L(A;\Lambda,\Gamma)\big)^p\right] &= L^d\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[BA^p];\Lambda,\Gamma\big)\\ &\quad + L^{d-1}\log L\ \mathfrak{W}_1\big(\operatorname{tr}_{\mathbb{C}^n}[BA^p]\,\mathfrak{U}(g_p;1);\partial\Lambda,\partial\Gamma\big)\\ &\quad + o(L^{d-1}\log L),\end{aligned} \tag{4.21}$$

as $L \to \infty$. Here, g_p is the monomial of degree p, the coefficients $\mathfrak{W}_0$ and $\mathfrak{W}_1$ are defined in (2.15) *and* (2.16)*, respectively, and we refer to* (2.17) *for the definition of the symbol $\mathfrak{U}$.*

Proof. We first give a proof in the case that Γ is unbounded, A is compactly supported in the second variable and B is not compactly supported in the second variable.

Let $R > 0$ such that the support of A in the second variable is contained in $B_R(0)$. By the definition of T_L we have

$$\begin{aligned}&\operatorname{Op}_L^l(B)\big(T_L(A;\Lambda,\Gamma)\big)^p\\ &\qquad = \operatorname{Op}_L^l(B)\mathbf{1}_\Lambda\operatorname{Op}_L(\mathbf{1}_\Gamma)\operatorname{Op}_L^l(A)\operatorname{Op}_L(\mathbf{1}_{B_R(0)})\operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda\big(T_L(A;\Lambda,\Gamma)\big)^{p-1}.\end{aligned} \tag{4.22}$$

Both Λ and $B_R(0)\cap\Gamma$ are bounded, therefore we can cover their closures with finitely many open balls such that Λ, respectively Γ, is represented by a basic domain denoted by Λ_j for $j \in \mathcal{J}$, respectively Γ_k for $k \in \mathcal{K}$, when restricted to any of such balls. Here, $\mathcal{J}, \mathcal{K} \subset \mathbb{N}$ are two finite index sets. We denote a partition of unity subordinate to the covering of Λ by $\{\phi_j\}_{j\in\mathcal{J}}$ and a partition of unity subordinate to the covering of $B_R(0)\cap\Gamma$ by $\{\psi_k\}_{k\in\mathcal{K}}$. By the construction of the coverings we have

$$\operatorname{Op}_L(\mathbf{1}_{B_R(0)})\operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda = \sum_{j\in\mathcal{J},\ k\in\mathcal{K}}\operatorname{Op}_L(\mathbf{1}_{B_R(0)\cap\Gamma})\operatorname{Op}_L^r(\phi_j\psi_k)\mathbf{1}_\Lambda. \tag{4.23}$$

We note that the symbol $\phi_j\psi_k$ of the right operator $\operatorname{Op}_L^r(\phi_j\psi_k)$ is to be understood as $\phi_j\psi_k$: $\mathbb{R}^d \times \mathbb{R}^d \ni (y,\xi) \mapsto \phi_j(y)\psi_k(\xi)$. As in (3.42) this is an abuse of notation and it is only clear from the definitions of the functions $\{\phi_j\}_{j\in\mathcal{J}}$ and $\{\psi_k\}_{k\in\mathcal{K}}$. With (4.23), we obtain

$$\begin{aligned}&\operatorname{Op}_L^l(B)\mathbf{1}_\Lambda\operatorname{Op}_L(\mathbf{1}_\Gamma)\operatorname{Op}_L^l(A)\operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda\\ &\qquad = \sum_{j\in\mathcal{J},\ k\in\mathcal{K}}\operatorname{Op}_L^l(B)\mathbf{1}_\Lambda\operatorname{Op}_L(\mathbf{1}_\Gamma)\operatorname{Op}_L^l(A)\operatorname{Op}_L(\mathbf{1}_\Gamma)\operatorname{Op}_L^r(\phi_j\psi_k)\mathbf{1}_\Lambda.\end{aligned} \tag{4.24}$$

We note that the symbol $\phi_j\psi_k$ is compactly supported in both variables. Therefore, for every $j \in \mathcal{J}$ and $k \in \mathcal{K}$, we can establish the following relations with the help of Lemmas 3.6 and 3.5

$$\operatorname{Op}_L(\mathbf{1}_\Gamma)\operatorname{Op}_L^r(\phi_j\psi_k) \sim \operatorname{Op}_L^r(\phi_j\psi_k)\operatorname{Op}_L(\mathbf{1}_\Gamma) \sim \operatorname{Op}_L^l(\phi_j\psi_k)\operatorname{Op}_L(\mathbf{1}_\Gamma),$$

$$\operatorname{Op}_L^l(A)\operatorname{Op}_L^l(\phi_j\psi_k) \sim \operatorname{Op}_L^l(A\phi_j\psi_k) \sim \operatorname{Op}_L^l(\phi_j\psi_k)\operatorname{Op}_L^l(A) \sim \operatorname{Op}_L^r(\phi_j\psi_k)\operatorname{Op}_L^l(A),$$

$$\mathbf{1}_\Lambda\operatorname{Op}_L^l(\phi_j\psi_k) \sim \operatorname{Op}_L^l(\phi_j\psi_k)\mathbf{1}_\Lambda. \tag{4.25}$$

Combining them yields

$$\begin{aligned}\operatorname{Op}_L^l(B)\big(T_L(A;\Lambda,\Gamma)\big)^p &\sim \sum_{j\in\mathcal{J},\, k\in\mathcal{K}} \operatorname{Op}_L^l(B)\operatorname{Op}_L^l(\phi_j\psi_k)\big(T_L(A;\Lambda,\Gamma)\big)^p \\ &\sim \sum_{j\in\mathcal{J},\, k\in\mathcal{K}} \operatorname{Op}_L^l(B_{j,k})\big(T_L(A;\Lambda,\Gamma)\big)^p, \end{aligned} \tag{4.26}$$

where the matrix-valued symbol $B_{j,k}$ is defined by $B_{j,k}(x,\xi) := B(x,\xi)\phi_j(x)\psi_k(\xi)$ for $x,\xi\in\mathbb{R}^d$. We note that the symbol $B_{j,k}$ is compactly supported in both variables and that

$$B_{j,k}|_{\Lambda\times\mathbb{R}^d} = B_{j,k}|_{\Lambda_j\times\mathbb{R}^d} \quad\text{and}\quad B_{j,k}|_{\mathbb{R}^d\times\Gamma} = B_{j,k}|_{\mathbb{R}^d\times\Gamma_k}. \tag{4.27}$$

Therefore, all the conditions of Lemma 4.2 are satisfied and we conclude

$$\operatorname{Op}_L^l(B)\big(T_L(A;\Lambda,\Gamma)\big)^p \sim \sum_{j\in\mathcal{J},\, k\in\mathcal{K}} \operatorname{Op}_L^l(B_{j,k}A^p)\big(T_L(\mathbb{1}_n;\Lambda_j,\Gamma_k)\big)^p. \tag{4.28}$$

Now both Λ_j and Γ_k are basic domains. Therefore, an application of Theorem 4.3 yields the asymptotic expansion

$$\begin{aligned}&\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\operatorname{Op}_L^l(B_{j,k}A^p)\big(T_L(\mathbb{1}_n;\Lambda_j,\Gamma_k)\big)^p\right] \\ &\quad= L^d\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[B_{j,k}A^p];\Lambda_j,\Gamma_k\big) + L^{d-1}\log L\,\mathfrak{W}_1\big(\operatorname{tr}_{\mathbb{C}^n}[B_{j,k}A^p]\,\mathfrak{A}(g_p;1);\partial\Lambda_j,\partial\Gamma_k\big) \\ &\qquad + o(L^{d-1}\log L),\end{aligned} \tag{4.29}$$

as $L\to\infty$. As Λ and Γ are locally represented by Λ_j and Γ_k, we can replace each occurrence of the basic domains by Λ respectively Γ. Using the linearity of the coefficients, we see that

$$\begin{aligned}&\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\sum_{j\in\mathcal{J},\, k\in\mathcal{K}} \operatorname{Op}_L^l(B_{j,k}A^p)\big(T_L(\mathbb{1}_n;\Lambda_j,\Gamma_k)\big)^p\Big] \\ &\qquad= L^d\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[BA^p];\Lambda,\Gamma\big) + L^{d-1}\log L\,\mathfrak{W}_1\big(\operatorname{tr}_{\mathbb{C}^n}[BA^p]\,\mathfrak{A}(g_p;1);\partial\Lambda,\partial\Gamma\big) \\ &\qquad\quad + o(L^{d-1}\log L),\end{aligned} \tag{4.30}$$

which concludes the proof in the case that A is compactly supported in the second variable.

If instead Γ is bounded and A is no longer compactly supported in the second variable, we cover the bounded set Γ directly. We obtain a finite index-set $\mathcal{K}'$ such that

$$\begin{aligned}&\operatorname{Op}_L^l(B)\mathbf{1}_\Lambda\operatorname{Op}_L(\mathbf{1}_\Gamma)\operatorname{Op}_L^l(A)\operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda \\ &\qquad= \sum_{j\in\mathcal{J},\, k\in\mathcal{K}'} \operatorname{Op}_L^l(B)\mathbf{1}_\Lambda\operatorname{Op}_L^l(\phi_j\psi_k)\operatorname{Op}_L(\mathbf{1}_\Gamma)\operatorname{Op}_L^l(A)\operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda.\end{aligned} \tag{4.31}$$

As the symbol $\phi_j\psi_k$ is again compactly supported in both variables, an application of Lemma 3.6 yields

$$\operatorname{Op}_L^l(B)\big(T_L(A;\Lambda,\Gamma)\big)^p \sim \sum_{j\in\mathcal{J},\, k\in\mathcal{K}'} \operatorname{Op}_L^l(B_{j,k})\big(T_L(A;\Lambda,\Gamma)\big)^p. \tag{4.32}$$

From here on, the proof continues as in the previous case, starting directly after (4.26).

In the third case, we assume that B is compactly supported in the second variable, Γ is not bounded and A is not compactly supported in the second variable. By the cyclic property of the trace, we have

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\operatorname{Op}_L^l(B)\big(T_L(A;\Lambda,\Gamma)\big)^p\right] = \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\mathbf{1}_\Lambda\operatorname{Op}_L^l(B)\big(T_L(A;\Lambda,\Gamma)\big)^p\right]. \tag{4.33}$$

As Λ is bounded, we find a smooth function $\phi \in C_c^\infty(\mathbb{R}^d)$ with $\phi|_\Lambda = 1$. Therefore, by Lemma 3.6 and (3.17), we obtain

$$\begin{aligned} \mathbf{1}_\Lambda \operatorname{Op}_L^l(B)\big(T_L(A;\Lambda,\Gamma)\big)^p &= \mathbf{1}_\Lambda \operatorname{Op}_L^l(\phi B)\big(T_L(A;\Lambda,\Gamma)\big)^p \\ &\sim \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Op}_L^l(\phi BA) \operatorname{Op}_L(\mathbf{1}_\Gamma)\big(T_L(A;\Lambda,\Gamma)\big)^{p-1}. \end{aligned} \tag{4.34}$$

We now choose $R > 0$ such that the support of B in the second variable is contained in $B_R(0)$ and cover the bounded sets Λ and $\Gamma \cap B_R(0)$ as in the first case. With this the operator on the right-hand side of (4.34) reads

$$\begin{aligned} &\sum_{j\in\mathcal{J},\, k\in\mathcal{K}} \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Op}_L^l(\phi BA) \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Op}_L^r(\phi_j\psi_k)\big(T_L(A;\Lambda,\Gamma)\big)^{p-1} \\ &\quad\sim \sum_{j\in\mathcal{J},\, k\in\mathcal{K}} \mathbf{1}_\Lambda \operatorname{Op}_L^l(\phi B\phi_j\psi_k) \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Op}_L^l(A) \operatorname{Op}_L(\mathbf{1}_\Gamma)\big(T_L(A;\Lambda,\Gamma)\big)^{p-1} \\ &\quad\sim \sum_{j\in\mathcal{J},\, k\in\mathcal{K}} \operatorname{Op}_L^l(B\phi_j\psi_k)\big(T_L(A;\Lambda,\Gamma)\big)^p, \end{aligned} \tag{4.35}$$

where we used Lemma 3.6, (3.14) and (3.16). From here on, the proof continues as in the first case, starting directly after (4.26).

This concludes the proof of all three cases and the proof of the theorem. □

4.3. Extension to more general Wiener–Hopf operators

In this section we generalise the results from Section 4.2 to treat more general jump discontinuities at the boundary $\partial\Gamma$ of the momentum region $\Gamma \subset \mathbb{R}^d$ with different matrix-valued symbols A_1 and A_2 on the inside, respectively outside. The non-commutativity of A_1 and A_2 represents an additional technical challenge in the proof of the next theorem for matrix-valued symbols as compared to the scalar case [Sob17, Thm. 5.2] . We recall the definitions of the Wiener–Hopf operators $D_L(A_1, A_2)$ and $G_L(A_1, A_2)$ in (2.30) and (2.31).

Theorem 4.5. *Let $p \in \mathbb{N}$, let $A_1, A_2 \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be matrix-valued symbols and assume A_2 to be compactly supported in the second variable. Let Λ be a bounded piece-wise C^1-admissible domain and Γ be a piece-wise C^3-admissible domain. We assume Γ to be bounded or A_1 to be compactly supported in the second variable. Then*

$$\begin{aligned} \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\big(D_L(A_1,A_2;\Lambda,\Gamma)\big)^p\right] &= L^d\big[\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[A_1^p];\Lambda,\Gamma\big) + \mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[A_2^p];\Lambda,\Gamma^c\big)\big] \\ &\quad + L^{d-1}\log L\ \mathfrak{W}_1\big(\mathfrak{U}(g_p;A_1,A_2);\partial\Lambda,\partial\Gamma\big) \\ &\quad + o(L^{d-1}\log L), \end{aligned} \tag{4.36}$$

as $L \to \infty$. Here, g_p is the monomial of degree p, the coefficients $\mathfrak{W}_0$ and $\mathfrak{W}_1$ are defined in (2.15) *and* (2.16)*, respectively, and we refer to* (2.32) *for the definition of the symbol $\mathfrak{U}$.*

Proof. We begin with a proof in the case that Γ is bounded and A_1 is not compactly supported in the second variable.

As Λ and Γ are bounded, we find real-valued functions $\phi, \psi \in C_c^\infty(\mathbb{R}^d)$ such that

$$\phi|_\Lambda = 1 \ \text{ and } \ \psi|_\Gamma = 1. \tag{4.37}$$

By construction we have $\mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma) = \mathbf{1}_\Lambda \operatorname{Op}_L^l(\phi\psi) \operatorname{Op}_L(\mathbf{1}_\Gamma)$. We rewrite

$$T_L(A_1;\Lambda,\Gamma) = \mathbf{1}_\Lambda \operatorname{Op}_L^l(\phi\psi) \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Op}_L^l(A_1) \operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda. \tag{4.38}$$

Using Lemmas 3.6 and 3.5, we obtain

$$\mathbf{1}_\Lambda \operatorname{Op}_L^l(\phi\psi) \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Op}_L^l(A_1) \operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda \sim \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Op}_L^l(\phi\psi A_1) \operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda. \tag{4.39}$$

As the symbol $\phi\psi A_1$ is compactly supported in both variables, further commutation yields

$$T_L(A_1;\Lambda,\Gamma) \sim \mathbf{1}_\Lambda \operatorname{Op}_L^l(\phi\psi A_1) \operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda = \mathbf{1}_\Lambda \operatorname{Op}_L^l(A_1) \operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda. \tag{4.40}$$

For the operator $T_L(A_2;\Lambda,\Gamma^c)$ we argue in a similar fashion. Let $\zeta \in C_c^\infty(\mathbb{R}^d)$ be a function such that ζ equals 1 on the support of A_2 in its second variable. We write

$$\begin{aligned} T_L(A_2;\Lambda,\Gamma^c) &= \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \operatorname{Op}_L^l(A_2) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \operatorname{Op}_L^r(\phi\zeta)\mathbf{1}_\Lambda \\ &\sim \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \operatorname{Op}_L^l(A_2\phi\zeta) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Lambda \\ &= \mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \operatorname{Op}_L^l(A_2\phi) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Lambda \\ &\sim \mathbf{1}_\Lambda \operatorname{Op}_L^l(A_2) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Lambda. \end{aligned} \tag{4.41}$$

Here, the commutation with $\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})$ is possible because $\operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) = \operatorname{Op}_L(\mathbf{1}_{(\overline{\Gamma})^c})$, as is explained in Remark 2.3. Combining (4.40), (4.41) and (4.40) for $A_1 - A_2$, we see that

$$D_L(A_1,A_2) = T_L(A_1;\Lambda,\Gamma) + T_L(A_2;\Lambda,\Gamma^c) \sim T_L(A_2;\Lambda,\mathbb{R}^d) + T_L(A_1 - A_2;\Lambda,\Gamma). \tag{4.42}$$

The next step is to compute the trace of $\big(D_L(A_1,A_2)\big)^p$ for $p \in \mathbb{N}$. The operators $T_L(A_2;\Lambda,\mathbb{R}^d)$ and $T_L(A_1 - A_2;\Lambda,\Gamma)$ do not even commute up to area terms because the matrix-valued symbols A_2 and $B := A_1 - A_2$ do not necessarily commute. Therefore, we need to be more careful than in the scalar-valued case. In order to write out the result, we use the expansion

$$(X+Y)^p = \sum_{k=0}^p \frac{1}{k!(p-k)!} \sum_{\pi \in \mathcal{S}_p} Z_{\pi(1)}^{(k)} \cdots Z_{\pi(p)}^{(k)} \tag{4.43}$$

for X and Y elements of an associative algebra and

$$Z_j^{(k)} := X \text{ if } j > k, \qquad Z_j^{(k)} := Y \text{ if } j \leqslant k, \qquad \text{for } k \in \{0,\dots,p\}, j \in \{1,\dots,p\}. \tag{4.44}$$

Here $\mathcal{S}_p$ denotes the symmetric group on the set $\{1,\dots,p\}$. Applying this expansion with $X = T_L(A_2;\Lambda,\mathbb{R}^d)$ and $Y = T_L(B;\Lambda,\Gamma)$, yields

$$\big(D_L(A_1,A_2)\big)^p \sim \sum_{k=0}^p \frac{1}{k!(p-k)!} \sum_{\pi \in \mathcal{S}_p} Z_{\pi(1)}^{(k)} \cdots Z_{\pi(p)}^{(k)}. \tag{4.45}$$

We note that $X = T_L(\phi A_2;\Lambda,\mathbb{R}^d)$, where the symbol ϕA_2 is compactly supported in both variables. The goal is to move all occurrences of $\operatorname{Op}_L^l(\phi A_2)$ and $\operatorname{Op}_L^l(B)$ to the left in order to apply Theorem 4.4 for the asymptotic evaluation of $\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\big(D_L(A_1,A_2)\big)^p\big]$. To this end, we introduce the symbols

$$C_j^{(k)} := A_2 \text{ if } j > k, \qquad C_j^{(k)} := B \text{ if } j \leqslant k, \qquad \text{for } k \in \{0,\dots,p\}, j \in \{1,\dots,p\}. \tag{4.46}$$

Since the symbol B is not necessarily supported in both variables, the established commutation results in Section 3.2 do not apply directly to it. For this reason we will treat the term with $k = p$ in (4.45) later, as it does not contain a factor $\operatorname{Op}_L^l(\phi A_2)$. For $k \in \{0,\dots,p-1\}$ such a factor is present, and Lemma 3.6 permits to commute the factor with $\mathbf{1}_\Lambda$ and $\operatorname{Op}_L(\mathbf{1}_\Gamma)$ up to area terms and Lemma 3.5 allows to merge it, up to area terms, with other factors $\operatorname{Op}_L^l(\phi A_2)$ or $\operatorname{Op}_L^l(B)$, the result being a left operator of a symbol that is compactly supported in both variables. In this way, we start with the rightmost factor of $\mathrm{Op}_L^l(\phi A_2)$ and move it to the right, thereby uniting it with all $\mathrm{Op}_L^l(B)$ to the right of it in a single Op_L^l. Subsequently moving this operator to the very left, we obtain

$$Z_{\pi(1)}^{(k)} \cdots Z_{\pi(p)}^{(k)} \sim \mathbf{1}_\Lambda \mathrm{Op}_L^l \Big(\phi^{p-k} C_{\pi(1)}^{(k)} \cdots C_{\pi(p)}^{(k)}\Big)\Big(\mathbf{1}_\Lambda \mathrm{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda\Big)^k \tag{4.47}$$

for $k \in \{0, \dots, p-1\}$. The factor $\mathbf{1}_\Lambda$ on the left is only relevant if $k = 0$, otherwise it can be absorbed in $\big(\mathbf{1}_\Lambda \mathrm{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda\big)^k$ up to area terms or via the cyclic property of the trace. Next, we claim that

$$\begin{aligned}
&\mathrm{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\big(D_L(A_1, A_2)\big)^p\big] \\
&\quad = L^d \mathfrak{W}_0\Big(\mathrm{tr}_{\mathbb{C}^n}[A_2^p]; \Lambda, \mathbb{R}^d\Big) \\
&\qquad + L^d \sum_{k=1}^p \frac{1}{k!(p-k)!} \sum_{\pi\in\mathcal{S}_p} \mathfrak{W}_0\Big(\mathrm{tr}_{\mathbb{C}^n}\big[C_{\pi(1)}^{(k)} \cdots C_{\pi(p)}^{(k)}\big]; \Lambda, \Gamma\Big) \\
&\qquad + L^{d-1}\log L \sum_{k=1}^p \frac{1}{k!(p-k)!} \sum_{\pi\in\mathcal{S}_p} \mathfrak{W}_1\Big(\mathrm{tr}_{\mathbb{C}^n}\big[C_{\pi(1)}^{(k)} \cdots C_{\pi(p)}^{(k)}\big]\, \mathfrak{U}(g_k; 1); \partial\Lambda, \partial\Gamma\Big) \\
&\qquad + o(L^{d-1}\log L),
\end{aligned} \tag{4.48}$$

as $L \to \infty$. The first line on the right-hand side arises from the direct computation of the term with $k = 0$ in (4.45) and (4.47). The terms with $k \in \{1, \dots, p-1\}$ in (4.45) and (4.47) give rise to the corresponding terms in the sums of the second and third line of (4.48) by applying Theorem 4.4 with B there given by $\phi^{p-k} C_{\pi(1)}^{(k)} \cdots C_{\pi(p)}^{(k)}$ and A there given by $\mathbb{1}_n$ (we recall that Γ is bounded). The terms with $k = p$ in the second and third line of (4.48) are obtained by applying Theorem 4.4 directly to the term with $k = p$ in (4.45) by choosing B in Theorem 4.4 as $\mathbb{1}_n$ and A in Theorem 4.4 as B from this proof.

In order to conclude the proof, it just remains to rewrite the terms on the right-hand side of (4.48). Adding the first two terms, we obtain

$$\begin{aligned}
&L^d\bigg(\mathfrak{W}_0\big(\mathrm{tr}_{\mathbb{C}^n}[A_2^p]; \Lambda, \mathbb{R}^d\big) + \sum_{k=1}^p \frac{1}{k!(p-k)!} \sum_{\pi\in\mathcal{S}_p} \mathfrak{W}_0\Big(\mathrm{tr}_{\mathbb{C}^n}\big[C_{\pi(1)}^{(k)} \cdots C_{\pi(p)}^{(k)}\big]; \Lambda, \Gamma\Big)\bigg) \\
&= \Big(\frac{L}{2\pi}\Big)^d \int_\Lambda \bigg(\int_{\mathbb{R}^d} \mathrm{tr}_{\mathbb{C}^n}[A_2^p(x,\xi)]\,\mathrm{d}\xi \\
&\qquad\qquad + \int_\Gamma \sum_{k=1}^p \frac{1}{k!(p-k)!} \sum_{\pi\in\mathcal{S}_p} \mathrm{tr}_{\mathbb{C}^n}\big[C_{\pi(1)}^{(k)} \cdots C_{\pi(p)}^{(k)}(x,\xi)\big]\,\mathrm{d}\xi\bigg)\mathrm{d}x \\
&= \Big(\frac{L}{2\pi}\Big)^d \int_\Lambda \int_{\mathbb{R}^d} \mathrm{tr}_{\mathbb{C}^n}\big[(A_2 + B\mathbf{1}_\Gamma)^p(x,\xi)\big]\,\mathrm{d}\xi\,\mathrm{d}x \\
&= L^d\Big(\mathfrak{W}_0\big(\mathrm{tr}_{\mathbb{C}^n}[A_1^p]; \Lambda, \Gamma\big) + \mathfrak{W}_0\big(\mathrm{tr}_{\mathbb{C}^n}[A_2^p]; \Lambda, \Gamma^c\big)\Big),
\end{aligned} \tag{4.49}$$

where we used the expansion (4.43) with $X = A_2$ and $Y = B\mathbf{1}_\Gamma$ in the second step. For the third term in (4.48), we need to evaluate

$$\sum_{k=1}^p \frac{1}{k!(p-k)!} \sum_{\pi\in\mathcal{S}_p} \mathrm{tr}_{\mathbb{C}^n}\big[C_{\pi(1)}^{(k)} \cdots C_{\pi(p)}^{(k)}\big]\, \mathfrak{U}(g_k; 1). \tag{4.50}$$

The definition of $\mathfrak{U}$ and linearity of the trace imply that (4.50) is equal to

$$\begin{aligned}
&\frac{1}{(2\pi)^2}\int_0^1 \frac{\sum_{k=1}^{p}\frac{1}{k!(p-k)!}\sum_{\pi\in\mathcal{S}_p}\operatorname{tr}_{\mathbb{C}^n}\big[C^{(k)}_{\pi(1)}\cdots C^{(k)}_{\pi(p)}\big](t^k-t)}{t(1-t)}\,\mathrm{d}t\\
&\quad=\frac{1}{(2\pi)^2}\int_0^1 \frac{\operatorname{tr}_{\mathbb{C}^n}\big[\sum_{k=0}^{p}\frac{1}{k!(p-k)!}\sum_{\pi\in\mathcal{S}_p}C^{(k)}_{\pi(1)}\cdots C^{(k)}_{\pi(p)}(t^k-t)-A_2^p(1-t)\big]}{t(1-t)}\,\mathrm{d}t\\
&\quad=\frac{1}{(2\pi)^2}\int_0^1 \frac{\operatorname{tr}_{\mathbb{C}^n}\big[(A_2+Bt)^p-(A_2+B)^p t-A_2^p(1-t)\big]}{t(1-t)}\,\mathrm{d}t,
\end{aligned}\tag{4.51}$$

where we used the expansion (4.43) twice in the last step. Inserting $B=A_1-A_2$, we obtain the expression

$$\frac{1}{(2\pi)^2}\int_0^1 \frac{\operatorname{tr}_{\mathbb{C}^n}\big[\big(A_1t+A_2(1-t)\big)^p-A_1^p t-A_2^p(1-t)\big]}{t(1-t)}\,\mathrm{d}t=\mathfrak{U}(g_p;A_1,A_2)\tag{4.52}$$

for (4.50). Together with the linearity of $\mathfrak{W}_1$, (4.49) and (4.48) we obtain the asymptotic formula

$$\begin{aligned}
\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\big(D_L(A_1,A_2)\big)^p\big]&=L^d\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[A_1^p];\Lambda,\Gamma\big)+L^d\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[A_2^p];\Lambda,\Gamma^c\big)\\
&\quad+L^{d-1}\log L\,\mathfrak{W}_1\big(\mathfrak{U}(g_p;A_1,A_2);\partial\Lambda,\partial\Gamma\big)\\
&\quad+o(L^{d-1}\log L),
\end{aligned}\tag{4.53}$$

as $L\to\infty$. This concludes the proof in the case that Γ is bounded.

If Γ is unbounded and both A_1 and A_2 are compactly supported in the second variable, we follow the same strategy with the following modifications. Applying the argument in (4.41) to both $T_L(A_1;\Lambda,\Gamma)$ and $T_L(A_2;\Lambda,\Gamma^c)$ we see that we have

$$D_L(A_1,A_2;\Lambda,\Gamma)=T_L(A_1;\Lambda,\Gamma)+T_L(A_2;\Lambda,\Gamma^c)\sim T_L(A_2;\Lambda,\mathbb{R}^d)+T_L(A_1-A_2;\Lambda,\Gamma),\tag{4.54}$$

as in (4.42). As the symbol A_2 is again compactly supported in the second variable, we again obtain (4.45) and (4.47) after an application of the expansion (4.43) and the commutation procedure from the previous case. In order to also obtain (4.48) in this case, we need to justify each of the applications of Theorem 4.4 with the appropriate assumptions. The first line on the right-hand side of (4.48) again arises from direct computation of the $k=0$ term. The terms with $k\in\{1,\dots,p-1\}$ in the second and third line, stem from an application of Theorem 4.4 on the corresponding terms in (4.45) and (4.47). We again apply Theorem 4.4 with $B=\phi^{p-k}C^{(k)}_{\pi(1)}\cdots C^{(k)}_{\pi(p)}$ and $A=\mathbb{1}_n$ which is justified, as the symbol B is compactly supported in the second variable. For the term with $k=p$, we apply Theorem 4.4 with $B=\mathbb{1}_n$ and A as $B=A_1-A_2$ from this proof. The latter symbol is compactly supported in the second variable, as both A_1 and A_2 are compactly supported in the second variable. From here on the proof continues as in the previous case.

This concludes the proof of the second case and with it the proof of the theorem. □

The following straightforward corollary extends the just obtained formula to the operator $G_L(A_1,A_2)$.

Corollary 4.6. *Let $p \in \mathbb{N}$, let A_1, A_2, Λ and Γ be as in Theorem* 4.5. *Then we obtain the following asymptotic formula*

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\big(G_L(A_1,A_2;\Lambda,\Gamma)\big)^p\big] = {} & L^d\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[(\operatorname{Re}A_1)^p];\Lambda,\Gamma\big)\\ & + L^d\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[(\operatorname{Re}A_2)^p];\Lambda,\Gamma^c\big)\\ & + L^{d-1}\log L\;\mathfrak{W}_1\big(\mathfrak{U}(g_p;\operatorname{Re}A_1,\operatorname{Re}A_2);\partial\Lambda,\partial\Gamma\big)\\ & + o(L^{d-1}\log L),\end{aligned}\tag{4.55}$$

as $L \to \infty$.

Proof. By the definition of G_L we have

$$\begin{aligned}G_L(A_1,A_2) - D_L(\operatorname{Re}A_1,\operatorname{Re}A_2) = {} & S_L(A_1;\Lambda,\Gamma) - T_L(\operatorname{Re}A_1;\Lambda,\Gamma)\\ & + S_L(A_2;\Lambda,\Gamma^c) - T_L(\operatorname{Re}A_2;\Lambda,\Gamma^c).\end{aligned}\tag{4.56}$$

As in (4.40) and (4.41), we can assume that our symbols are compactly supported in both variables. Using that $\big(\operatorname{Op}_L^l(\operatorname{Re}A_1)\big)^* = \operatorname{Op}_L^r(\operatorname{Re}A_1)$ and applying Lemma 3.5, we see that

$$\big\|S_L(A_1;\Lambda,\Gamma) - T_L(\operatorname{Re}A_1;\Lambda,\Gamma)\big\|_1 \leqslant \frac{1}{2}\,\big\|\operatorname{Op}_L^r(\operatorname{Re}A_1) - \operatorname{Op}_L^l(\operatorname{Re}A_1)\big\|_1 \leqslant CL^{d-1}.\tag{4.57}$$

Also applying this procedure with A_2 and Γ^c, we obtain

$$G_L(A_1,A_2) \sim D_L(\operatorname{Re}A_1,\operatorname{Re}A_2).\tag{4.58}$$

Iterative use of (4.58) together with Hölder's inequality and the fact that $G_L(A_1,A_2)$ is uniformly bounded in L, yields

$$\big(G_L(A_1,A_2)\big)^p \sim \big(D_L(\operatorname{Re}A_1,\operatorname{Re}A_2)\big)^p.\tag{4.59}$$

It just remains to apply Theorem 4.5 to obtain the desired asymptotic formula. □

Sometimes it is useful to consider domains Λ which are not bounded themselves but only have bounded complement. In this case, the volume term is not well-defined but, for symbols which only depend on momentum space, we still obtain the following consequence of Theorem 4.5.

Corollary 4.7. *Let $p \in \mathbb{N}$, let A_1, A_2 and Γ be as in Theorem* 4.5. *Further assume that A_1 and A_2 are only supported in the single variable ξ. Let Λ be a piece-wise C^1-admissible domain such that Λ^c is bounded. Then we have*

$$\begin{aligned}\lim_{L\to\infty}\frac{\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\big(G_L(A_1,A_2;\Lambda,\Gamma)\big)^p - D_L\big((\operatorname{Re}A_1)^p,(\operatorname{Re}A_2)^p;\Lambda,\Gamma\big)\big]}{L^{d-1}\log L}&\\ = \mathfrak{W}_1\big(\mathfrak{U}(g_p;\operatorname{Re}A_1,\operatorname{Re}A_2);\partial\Lambda,\partial\Gamma\big).&\end{aligned}\tag{4.60}$$

Proof. Define a real-valued smooth function $\phi \in C_c^\infty(\mathbb{R}^d)$ with $\phi|_{\Lambda^c} = 1$. We note that $(1-\phi^p)\mathbf{1}_{\Lambda^c} = 0$ and therefore

$$(1-\phi^p)\mathbf{1}_\Lambda = (1-\phi^p)(\mathbf{1}_\Lambda + \mathbf{1}_{\Lambda^c}) = (1-\phi^p)\mathbf{1}_{\mathbb{R}^d}.\tag{4.61}$$

Next, we claim that $\phi G_L(A_1,A_2;\Lambda,\Gamma) \sim G_L(\phi A_1,\phi A_2;\Lambda,\Gamma) \sim G_L(A_1,A_2;\Lambda,\Gamma)\phi$. To see this, we note that by (4.40) and (4.41) we have

$$G_L(A_1,A_2;\Lambda,\Gamma) \sim \mathbf{1}_\Lambda\big[\operatorname{Re}\operatorname{Op}_L^l(\operatorname{Re}A_1)\operatorname{Op}_L(\mathbf{1}_\Gamma) + \operatorname{Re}\operatorname{Op}_L^l(\operatorname{Re}A_2)\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\big]\mathbf{1}_\Lambda\tag{4.62}$$

and therefore

$$\begin{aligned}\phi G_L(A_1, A_2; \Lambda, \Gamma) &\sim \mathbf{1}_\Lambda \big[\operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} \phi A_1) \operatorname{Op}_L(\mathbf{1}_\Gamma) + \operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} \phi A_2) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \big] \mathbf{1}_\Lambda \\ &\sim G_L(\phi A_1, \phi A_2; \Lambda, \Gamma). \end{aligned} \tag{4.63}$$

Choosing $\zeta \in C_c^\infty(\mathbb{R}^d)$ in such a way that ζ equals 1 on the support of A_2 in the second variable, as well as on the intersection of Γ with the support of A_1 in the second variable, we obtain

$$\begin{aligned}&\mathbf{1}_\Lambda \big[\operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} \phi A_1) \operatorname{Op}_L(\mathbf{1}_\Gamma) + \operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} \phi A_2) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \big] \mathbf{1}_\Lambda \\ &\qquad = \mathbf{1}_\Lambda \big[\operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} \phi A_1 \zeta) \operatorname{Op}_L(\mathbf{1}_\Gamma) + \operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} \phi A_2 \zeta) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \big] \mathbf{1}_\Lambda \\ &\qquad \sim \mathbf{1}_\Lambda \big[\operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} A_1) \operatorname{Op}_L(\mathbf{1}_\Gamma) + \operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} A_2) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \big] \operatorname{Op}_L^r(\phi\zeta) \mathbf{1}_\Lambda \\ &\qquad = \mathbf{1}_\Lambda \big[\operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} A_1) \operatorname{Op}_L(\mathbf{1}_\Gamma) + \operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} A_2) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \big] \mathbf{1}_\Lambda \phi \\ &\qquad \sim G_L(A_1, A_2; \Lambda, \Gamma) \phi. \end{aligned} \tag{4.64}$$

Here, we used Lemma 3.6 and (3.14) in the second step. Iterating this procedure, we see that, for every $p \in \mathbb{N}$, we have

$$\phi^p \big(G_L(A_1, A_2; \Lambda, \Gamma) \big)^p \sim \big(G_L(\phi A_1, \phi A_2; \Lambda, \Gamma) \big)^p \tag{4.65}$$

and

$$\begin{aligned}&(1 - \phi^p) \big(G_L(A_1, A_2; \Lambda, \Gamma) \big)^p - (1 - \phi^p) D_L \big((\operatorname{Re} A_1)^p, (\operatorname{Re} A_2)^p; \Lambda, \Gamma \big) \\ &\qquad \sim (1 - \phi^p) \big(G_L(A_1, A_2; \mathbb{R}^d, \Gamma) \big)^p - (1 - \phi^p) D_L \big((\operatorname{Re} A_1)^p, (\operatorname{Re} A_2)^p; \mathbb{R}^d, \Gamma \big) = 0, \end{aligned} \tag{4.66}$$

where we used (4.61) and the fact that A_1 and A_2 only depend on momentum space in the last equality. Combining (4.65) and (4.66), we conclude that

$$\begin{aligned}&\big(G_L(A_1, A_2; \Lambda, \Gamma) \big)^p - D_L \big((\operatorname{Re} A_1)^p, (\operatorname{Re} A_2)^p; \Lambda, \Gamma \big) \\ &\qquad \sim \big(G_L(\phi A_1, \phi A_2; \Lambda, \Gamma) \big)^p - D_L \big((\phi \operatorname{Re} A_1)^p, (\phi \operatorname{Re} A_2)^p; \Lambda, \Gamma \big). \end{aligned} \tag{4.67}$$

Due to the presence of ϕ in both symbols we can, up to area terms, treat Λ as a bounded domain, and Corollary 4.6 yields

$$\begin{aligned}&\lim_{L \to \infty} \frac{\operatorname{tr}_{L^2(\mathbb{R}^d) \otimes \mathbb{C}^n} \big[\big(G_L(\phi A_1, \phi A_2; \Lambda, \Gamma) \big)^p - D_L \big((\phi \operatorname{Re} A_1)^p, (\phi \operatorname{Re} A_2)^p; \Lambda, \Gamma \big) \big]}{L^{d-1} \log L} \\ &\qquad = \mathfrak{W}_1 \big(\mathfrak{U}(g_p; \phi \operatorname{Re} A_1, \phi \operatorname{Re} A_2); \partial\Lambda, \partial\Gamma \big), \end{aligned} \tag{4.68}$$

where we used the fact that

$$\begin{aligned}&\operatorname{tr}_{L^2(\mathbb{R}^d) \otimes \mathbb{C}^n} \big[D_L \big((\phi \operatorname{Re} A_1)^p, (\phi \operatorname{Re} A_2)^p; \Lambda, \Gamma \big) \big] \\ &\qquad = L^d \mathfrak{W}_0 \big(\operatorname{tr}_{\mathbb{C}^n} [(\operatorname{Re} A_1)^p]; \Lambda, \Gamma \big) + L^d \mathfrak{W}_0 \big(\operatorname{tr}_{\mathbb{C}^n} [(\operatorname{Re} A_2)^p]; \Lambda, \Gamma^c \big) \end{aligned} \tag{4.69}$$

which follows by direct integration of the integral kernel along the diagonal. As $\phi|_{\partial\Lambda} = 1$, we obtain the desired result. □

4.4. Closing the asymptotics: Analytic functions

We now want to establish the asymptotic expansion from Theorem 4.5 for more general functions than polynomials. In the case of a non-self-adjoint operator, we can only extend this to analytic functions. For self-adjoint operators more general functions are accessible.

We consider functions g with $g(0) = 0$ which are analytic in a disc $B_R(0) \subset \mathbb{C}$ about the origin with sufficiently large radius $R > 0$, i.e. there exist $\omega_m \in \mathbb{C}, m \in \mathbb{N}$, such that

$$g(z) = \sum_{m\in\mathbb{N}} \omega_m z^m, \tag{4.70}$$

for all $z \in B_R(0)$.

The trace of $D_L(g(A_1), g(A_2))$ can be computed explicitly and coincides (up to area terms) with the expected volume term.

Lemma 4.8. *Let $A_1, A_2 \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be matrix-valued symbols with A_2 being compactly supported in the second variable. Further, let Λ and Γ be bounded admissible domains. Then for any function g analytic in a disc $B_R(0) \subset \mathbb{C}$ of radius $R > \|\operatorname{Op}_L^l(A_1)\| + \|\operatorname{Op}_L^l(A_2)\|$ with $g(0) = 0$, we have*

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[D_L\big(g(A_1), g(A_2)\big)\right] = L^d\Big[&\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[g(A_1)]; \Lambda, \Gamma\big) + \mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[g(A_2)]; \Lambda, \Gamma^c\big)\Big]\\ &+ O(L^{d-1}),\end{aligned} \tag{4.71}$$

as $L \to \infty$.

Proof. Let $\phi, \psi \in C_c^\infty(\mathbb{R}^d)$ be as in (4.37), i.e. $\phi|_\Lambda = 1$ and $\psi|_\Gamma = 1$. First note that the function g being analytic guarantees that $g(A_j) \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ is a well-defined symbol for $j \in \{1, 2\}$. Further the property $g(0) = 0$ ensures that these symbols are again compactly supported whenever the corresponding symbol A_j is compactly supported. Therefore, the previous results (4.40) and (4.41) on C_b^∞-symbols apply and we obtain

$$D_L\big(g(A_1), g(A_2)\big) \sim \mathbf{1}_\Lambda \operatorname{Op}_L^l\big(g(A_1)\phi\psi\big) \operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda + \mathbf{1}_\Lambda \operatorname{Op}_L^l\big(g(A_2)\phi\big) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Lambda. \tag{4.72}$$

The trace of the right-hand side of (4.72) can be computed explicitly by integrating its kernel along the diagonal which yields

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}&\Big[\mathbf{1}_\Lambda \operatorname{Op}_L^l\big(g(A_1)\phi\psi\big) \operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda + \mathbf{1}_\Lambda \operatorname{Op}_L^l\big(g(A_2)\phi\big) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Lambda\Big]\\ &= L^d\Big[\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[g(A_1)]; \Lambda, \Gamma\big) + \mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[g(A_2)]; \Lambda, \Gamma^c\big)\Big].\end{aligned} \tag{4.73}$$

□

The crucial remaining step, in order to close the asymptotics, is to estimate the following trace norm

$$\big\|g\big(D_L(A_1, A_2)\big) - D_L\big(g(A_1), g(A_2)\big)\big\|_1 \tag{4.74}$$

and see that it only gives rise to an enhanced area term with coefficient depending on the function g. We divide this task into several steps and begin by reducing the question to symbols which are compactly supported in both variables. For some of the steps we will need a large radius of convergence. In order to define it, we first define the radius

$$t_A := \sup_{L\geqslant 1} \|\operatorname{Op}_L^l(A)\| + \mathbf{N}^{(d+1,d+2)}(A), \tag{4.75}$$

for a single matrix-valued symbol $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$, where $\mathbf{N}^{(d+1,d+2)}(A)$ is defined in (2.23).

Lemma 4.9. *Let $A_1, A_2 \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be matrix-valued symbols with A_2 being compactly supported in the second variable. Further, let Λ and Γ be bounded admissible domains. Then there exist symbols $B_1, B_2 \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$, compactly supported in both variables and with*

$$(A_1 - B_1)\big|_{\Lambda\times\Gamma} = 0, \qquad (A_2 - B_2)\big|_{\Lambda\times\mathbb{R}^d} = 0, \tag{4.76}$$

such that for any function g analytic in a disc $B_R(0) \subset \mathbb{C}$ of radius

$$R > t_0 := t_{A_1} + t_{A_2} + t_{B_1} + t_{B_2}, \tag{4.77}$$

with $g(0) = 0$, we have

$$D_L\big(g(A_1), g(A_2)\big) \sim D_L\big(g(B_1), g(B_2)\big) \tag{4.78}$$

and

$$g\big(D_L(A_1, A_2)\big) \sim g\big(D_L(B_1, B_2)\big). \tag{4.79}$$

Proof. Let $L \geqslant 1$. We find the compactly supported symbols by introducing smooth cut-off functions in the same way as in Lemma 4.8: Let $\phi, \psi \in C_c^\infty(\mathbb{R}^d)$ be as in (4.37) and define $B_1 := A_1\phi\psi$ and $B_2 := A_2\phi$. As in (4.72) we obtain

$$D_L\big(g(A_1), g(A_2)\big) \sim \mathbf{1}_\Lambda \operatorname{Op}_L^l\big(g(A_1)\phi\psi\big)\operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda + \mathbf{1}_\Lambda \operatorname{Op}_L^l\big(g(A_2)\phi\big)\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Lambda. \tag{4.80}$$

Since $\phi|_\Lambda = 1$ and $\psi|_\Gamma = 1$, we have

$$\begin{aligned}
\mathbf{1}_\Lambda \operatorname{Op}_L^l\big(g(A_1)\phi\psi\big)&\operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda + \mathbf{1}_\Lambda \operatorname{Op}_L^l\big(g(A_2)\phi\big)\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Lambda \\
&= \mathbf{1}_\Lambda \operatorname{Op}_L^l\big(g(B_1)\big)\operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda + \mathbf{1}_\Lambda \operatorname{Op}_L^l\big(g(B_2)\big)\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Lambda \\
&\sim D_L\big(g(B_1), g(B_2)\big),
\end{aligned} \tag{4.81}$$

where we used Lemma 3.6 in the last step. This proves (4.78).

In order to prove (4.79), we first note that

$$D_L(A_1, A_2) \sim D_L(B_1, B_2), \tag{4.82}$$

by setting $g = 1$ in (4.78). We now need to calculate the trace norm $\|(D_L(A_1, A_2))^m - (D_L(B_1, B_2))^m\|_1$ for arbitrary $m \in \mathbb{N}$. We note that the case $m = 0$ need not be considered here, due to $g(0) = 0$. Repeatedly applying (4.82) together with Hölder's inequality and the fact that $D_L(A_1, A_2)$ and $D_L(B_1, B_2)$ are bounded uniformly in L by t_0, we obtain

$$\big\|\big(D_L(A_1, A_2)\big)^m - \big(D_L(B_1, B_2)\big)^m\big\|_1 \leqslant L^{d-1}Cmt_0^{m-1}, \tag{4.83}$$

where the constant C depends neither on m nor L. Therefore, using the notation of (4.70), we obtain

$$\begin{aligned}
\big\|g\big(D_L(A_1, A_2)\big) - g\big(D_L(B_1, B_2)\big)\big\|_1 &= \Bigg\|\sum_{m=1}^\infty \omega_m\Big\{\big(D_L(A_1, A_2)\big)^m - \big(D_L(B_1, B_2)\big)^m\Big\}\Bigg\|_1 \\
&\leqslant L^{d-1}C\sum_{m=1}^\infty m|\omega_m|t_0^{m-1} \leqslant L^{d-1}C',
\end{aligned} \tag{4.84}$$

as g is analytic in $B_R(0)$. □

The next Lemma [Sob13, Lem. 12.1] deals with the projections in the operator D_L.

Lemma 4.10. *Let X be a trace-class operator in a separable Hilbert space $\mathcal{H}$. Let P be an orthogonal projection in $\mathcal{H}$ and g be as in* (4.70)*, a function that is analytic in a disc $B_R(0) \subset \mathbb{C}$ of radius $R > \|X\|$. Then we have*

$$\|g(PXP) - Pg(X)P\|_1 \leqslant g^{|1|}(\|X\|)\|PX(\mathbb{1}_\mathcal{H} - P)\|_1, \tag{4.85}$$

where

$$g^{|1|}(z) := \sum_{m=2}^\infty (m-1)|\omega_m|z^{m-1}, \qquad z \in B_R(0). \tag{4.86}$$

The next result deals with interchanging the test function g and the left-operator Op_L^l.

Lemma 4.11. *Let $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be a matrix-valued symbol with compact support in both variables and let g be a function that is analytic in a disc of radius $R > t_A$ about the origin and such that $g(0) = 0$. Then we have*

$$g\big(\operatorname{Op}_L^l(A)\big) \sim \operatorname{Op}_L^l\big(g(A)\big). \tag{4.87}$$

The radius t_A is defined in (4.75).

Proof. Let $L \geqslant 1$. It suffices to show

$$\big\|\big(\operatorname{Op}_L^l(A)\big)^m - \operatorname{Op}_L^l(A^m)\big\|_1 \leqslant DL^{d-1}(m-1)^{2(d+2)}t_A^{m-1}, \tag{4.88}$$

for every $m \in \mathbb{N}$ with the finite constant $D := C\mathbf{N}^{(d+1,d+2)}(A)$, where the constant C does not depend on L and m and is specified below (4.92). Indeed, the power-series expansion (4.70) of g then yields

$$\begin{aligned}\big\|g\big(\operatorname{Op}_L^l(A)\big) - \operatorname{Op}_L^l\big(g(A)\big)\big\|_1 &= \Big\|\sum_{m=1}^\infty \omega_m\Big\{\big(\operatorname{Op}_L^l(A)\big)^m - \operatorname{Op}_L^l(A^m)\Big\}\Big\|_1\\ &\leqslant DL^{d-1}\sum_{m=1}^\infty |\omega_m|(m-1)^{2(d+2)}t_A^{m-1},\end{aligned} \tag{4.89}$$

which gives a finite constant, as g is analytic in a disc of sufficiently large radius. We prove (4.88) by induction on m.

For $m = 1$, there is nothing to prove in (4.88). Now, suppose (4.88) holds for $m \in \mathbb{N}$. In order to prove (4.88) for $m+1$, we estimate

$$\begin{aligned}\big\|\big(\operatorname{Op}_L^l(A)\big)^{m+1} - \operatorname{Op}_L^l(A^{m+1})\big\|_1 &\leqslant \big\|\big(\operatorname{Op}_L^l(A)\big)^{m+1} - \operatorname{Op}_L^l(A^m)\operatorname{Op}_L^l(A)\big\|_1\\ &\quad + \big\|\operatorname{Op}_L^l(A^m)\operatorname{Op}_L^l(A) - \operatorname{Op}_L^l(A^{m+1})\big\|_1.\end{aligned} \tag{4.90}$$

For the first term, we use the induction hypothesis and Hölder's inequality

$$\begin{aligned}\big\|\big(\operatorname{Op}_L^l(A)\big)^{m+1} - \operatorname{Op}_L^l(A^m)\operatorname{Op}_L^l(A)\big\|_1 &\leqslant DL^{d-1}(m-1)^{2(d+2)}t_A^{m-1}\|\operatorname{Op}_L^l(A)\|\\ &\leqslant DL^{d-1}m^{2(d+2)}t_A^m.\end{aligned} \tag{4.91}$$

The second term is treated with Inequality (3.28) applied to the symbols A^m and A

$$\begin{aligned}\big\|\operatorname{Op}_L^l(A^m)\operatorname{Op}_L^l(A) - \operatorname{Op}_L^l(A^{m+1})\big\|_1 &\leqslant CL^{d-1}\mathbf{N}^{(d+1,d+2)}(A^m)\,\mathbf{N}^{(d+1,d+2)}(A)\\ &= DL^{d-1}\mathbf{N}^{(d+1,d+2)}(A^m).\end{aligned} \tag{4.92}$$

Therefore, it suffices to find an estimate for $\mathbf{N}^{(d+1,d+2)}(A^m)$. It follows from the definition (2.23) of the symbol norm that

$$\mathbf{N}^{(d+1,d+2)}(A^m) \leqslant m^{2(d+2)}\big(\mathbf{N}^{(d+1,d+2)}(A)\big)^m \leqslant m^{2(d+2)}t_A^m. \tag{4.93}$$

Inserting (4.93) into (4.92), adding (4.91) and using once again the definition (4.75) of t_A, we conclude the proof of the induction step. □

We now combine the previous results in order to obtain the desired estimate for (4.74).

Lemma 4.12. *Let $A_1, A_2 \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be matrix-valued symbols with A_2 being compactly supported in the second variable. Further, let Λ and Γ be bounded admissible domains. For any function g analytic in a disc of radius $R > t_0$ with $g(0) = 0$, there exist constants $C_1, C_2 > 0$, independent of L with C_1 also independent of g, such that*

$$\big\|g\big(D_L(A_1,A_2)\big) - D_L\big(g(A_1), g(A_2)\big)\big\|_1 \leqslant C_1 g^{|1|}(t_0)L^{d-1}\log L + C_2L^{d-1}, \tag{4.94}$$

for every $L \geqslant 2$. The radius t_0 is defined in (4.77) *and* (4.75).

Proof. Let $L \geqslant 2$. As Lemma 4.9 yields

$$g\big(D_L(A_1,A_2)\big) \sim g\big(D_L(B_1,B_2)\big) \tag{4.95}$$

and

$$D_L\big(g(A_1),g(A_2)\big) \sim D_L\big(g(B_1),g(B_2)\big), \tag{4.96}$$

it suffices to show (4.94) with A_1 and A_2 replaced by the compactly supported symbols B_1 and B_2. We do this, starting with the operator $g(D_L(B_1,B_2))$ on the left-hand side.

Lemma 4.10 applied to $\mathrm{Op}_L(\mathbf{1}_\Gamma)\,\mathrm{Op}_L^l(B_1)\,\mathrm{Op}_L(\mathbf{1}_\Gamma) + \mathrm{Op}_L(\mathbf{1}_{\Gamma^c})\,\mathrm{Op}_L^l(B_2)\,\mathrm{Op}_L(\mathbf{1}_{\Gamma^c})$ and $\mathbf{1}_\Lambda$, combined with the commutator estimate from Lemma 3.8, yields

$$\begin{aligned}
&\Big\| g\big(D_L(B_1,B_2)\big) - \mathbf{1}_\Lambda\, g\Big(\mathrm{Op}_L(\mathbf{1}_\Gamma)\,\mathrm{Op}_L^l(B_1)\,\mathrm{Op}_L(\mathbf{1}_\Gamma) + \mathrm{Op}_L(\mathbf{1}_{\Gamma^c})\,\mathrm{Op}_L^l(B_2)\,\mathrm{Op}_L(\mathbf{1}_{\Gamma^c})\Big)\mathbf{1}_\Lambda\Big\|_1 \\
&\quad\leqslant g^{|1|}(t_0)\Big(\big\|\mathbf{1}_\Lambda\,\mathrm{Op}_L(\mathbf{1}_\Gamma)\,\mathrm{Op}_L^l(B_1)\,\mathrm{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_{\Lambda^c}\big\|_1 + \big\|\mathbf{1}_\Lambda\,\mathrm{Op}_L(\mathbf{1}_{\Gamma^c})\,\mathrm{Op}_L^l(B_2)\,\mathrm{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_{\Lambda^c}\big\|_1\Big) \\
&\quad\leqslant C_1 g^{|1|}(t_0)\, L^{d-1}\log L.
\end{aligned} \tag{4.97}$$

Here, C_1 is already the constant from (4.94). For its independence of L we refer to Lemma 3.8. The power series expansion of the function g implies

$$\begin{aligned}
&g\Big(\mathrm{Op}_L(\mathbf{1}_\Gamma)\,\mathrm{Op}_L^l(B_1)\,\mathrm{Op}_L(\mathbf{1}_\Gamma) + \mathrm{Op}_L(\mathbf{1}_{\Gamma^c})\,\mathrm{Op}_L^l(B_2)\,\mathrm{Op}_L(\mathbf{1}_{\Gamma^c})\Big) \\
&\qquad = g\big(\mathrm{Op}_L(\mathbf{1}_\Gamma)\,\mathrm{Op}_L^l(B_1)\,\mathrm{Op}_L(\mathbf{1}_\Gamma)\big) + g\big(\mathrm{Op}_L(\mathbf{1}_{\Gamma^c})\,\mathrm{Op}_L^l(B_2)\,\mathrm{Op}_L(\mathbf{1}_{\Gamma^c})\big).
\end{aligned} \tag{4.98}$$

Applying Lemma 4.10 to $\mathrm{Op}_L^l(B_1)$ and $\mathrm{Op}_L(\mathbf{1}_\Gamma)$, followed by Lemma 3.8, yields

$$\begin{aligned}
&\big\| g\big(\mathrm{Op}_L(\mathbf{1}_\Gamma)\,\mathrm{Op}_L^l(B_1)\,\mathrm{Op}_L(\mathbf{1}_\Gamma)\big) - \mathrm{Op}_L(\mathbf{1}_\Gamma) g\big(\mathrm{Op}_L^l(B_1)\big)\,\mathrm{Op}_L(\mathbf{1}_\Gamma)\big\|_1 \\
&\qquad \leqslant g^{|1|}(t_0)\big\|\mathrm{Op}_L(\mathbf{1}_\Gamma)\,\mathrm{Op}_L^l(B_1)\,\mathrm{Op}_L(\mathbf{1}_{\Gamma^c})\big\|_1 \leqslant C L^{d-1}.
\end{aligned} \tag{4.99}$$

Applying Lemma 4.10 again to $\mathrm{Op}_L^l(B_2)$ and $\mathrm{Op}_L(\mathbf{1}_{\Gamma^c})$, we conclude

$$\begin{aligned}
&\mathbf{1}_\Lambda\, g\Big(\mathrm{Op}_L(\mathbf{1}_\Gamma)\,\mathrm{Op}_L^l(B_1)\,\mathrm{Op}_L(\mathbf{1}_\Gamma) + \mathrm{Op}_L(\mathbf{1}_{\Gamma^c})\,\mathrm{Op}_L^l(B_2)\,\mathrm{Op}_L(\mathbf{1}_{\Gamma^c})\Big)\mathbf{1}_\Lambda \\
&\qquad \sim \mathbf{1}_\Lambda\Big(\mathrm{Op}_L(\mathbf{1}_\Gamma) g\big(\mathrm{Op}_L^l(B_1)\big)\,\mathrm{Op}_L(\mathbf{1}_\Gamma) + \mathrm{Op}_L(\mathbf{1}_{\Gamma^c}) g\big(\mathrm{Op}_L^l(B_2)\big)\,\mathrm{Op}_L(\mathbf{1}_{\Gamma^c})\Big)\mathbf{1}_\Lambda.
\end{aligned} \tag{4.100}$$

Finally, Lemma 4.11 yields

$$\mathbf{1}_\Lambda\,\mathrm{Op}_L(\mathbf{1}_\Gamma) g\big(\mathrm{Op}_L^l(B_1)\big)\,\mathrm{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda \sim T_L\big(g(B_1);\Lambda,\Gamma\big), \tag{4.101}$$

as well as

$$\mathbf{1}_\Lambda\,\mathrm{Op}_L(\mathbf{1}_{\Gamma^c}) g\big(\mathrm{Op}_L^l(B_2)\big)\,\mathrm{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Lambda \sim T_L\big(g(B_2);\Lambda,\Gamma^c\big). \tag{4.102}$$

The claim follows, because $D_L\big(g(B_1),g(B_2);\Lambda,\Gamma\big) = T_L\big(g(B_1);\Lambda,\Gamma\big) + T_L\big(g(B_2);\Lambda,\Gamma^c\big)$. □

We also need the following estimate for the coefficient $\mathfrak{W}_1$.

Lemma 4.13. *Let $A_1, A_2 \in C_b^\infty(\mathbb{R}^d\times\mathbb{R}^d,\mathbb{C}^{n\times n})$ be matrix-valued symbols. Let the function g be analytic in a disc of radius $R > t_0$ with $g(0)=0$. Let $\partial\Lambda$ and $\partial\Gamma$ have finite $(d-1)$-dimensional surface measure induced by Lebesgue measure on $\mathbb{R}^d$. Then*

$$\big|\mathfrak{W}_1\big(\mathfrak{U}(g;A_1,A_2);\partial\Lambda,\partial\Gamma\big)\big| \leqslant \frac{|\partial\Lambda||\partial\Gamma|}{(2\pi)^2}\, t_0 g^{|1|}(t_0). \tag{4.103}$$

The radius t_0 is defined in (4.77) *and* (4.75).

Proof. As the surface measure of $\partial\Lambda$ and $\partial\Gamma$ is finite, it suffices to show

$$\sup_{(x,\xi)\in\partial\Lambda\times\partial\Gamma}\Big|\big(\mathfrak{U}(g;A_1,A_2)\big)(x,\xi)\Big| \leqslant \frac{t_0}{(2\pi)^2}\, g^{|1|}(t_0). \tag{4.104}$$

To start with, we choose the test function g as a monomial of order $m\in\mathbb{N}$ and work towards a pointwise estimate for the function

$$\begin{aligned}(2\pi)^2\mathfrak{U}(g_m;A_1,A_2) &= \int_0^1 \frac{\operatorname{tr}_{\mathbb{C}^n}\left[\big(A_1t+A_2(1-t)\big)^m - A_1^m t - A_2^m(1-t)\right]}{t(1-t)}\,\mathrm{d}t\\ &= \operatorname{tr}_{\mathbb{C}^n}\Bigg[\int_0^1\Bigg(\frac{(A_1t)^m - A_1^m t}{t(1-t)} + \frac{\big(A_2(1-t)\big)^m - A_2^m(1-t)}{t(1-t)}\\ &\qquad + \sum_{k=1}^{m-1}\frac{1}{k!(m-k)!}\sum_{\pi\in\mathcal{S}_m} Z^{(k)}_{\pi(1)}\cdots Z^{(k)}_{\pi(m)}\,\frac{t^k(1-t)^{m-k}}{t(1-t)}\Bigg)\mathrm{d}t\Bigg],\end{aligned} \tag{4.105}$$

where the $Z_j^{(k)}$, for $j\in\{1,\dots,m\}$ and $k\in\{1,\dots,m-1\}$, are defined as in the expansion (4.43) with $X=A_2$, $Y=A_1$ and $p=m$. The integral $\int_0^1\frac{t^k(1-t)^{m-k}}{t(1-t)}\,\mathrm{d}t$ is bounded from above by 1 for every $k\in\{1,\dots,m-1\}$. For the first integrand on the right-hand side of (4.105), we estimate $|\int_0^1\frac{t^m-t}{t(1-t)}\,\mathrm{d}t| = \int_0^1\sum_{j=0}^{m-2}t^j\,\mathrm{d}t \leqslant m-1$. By a change of variables, we also have $|\int_0^1\frac{(1-t)^m-(1-t)}{t(1-t)}\,\mathrm{d}t|\leqslant m-1$ for the second integrand. Introducing the norm

$$\|A\|_{\infty,1} := \sup_{(x,\xi)\in\partial\Lambda\times\partial\Gamma}\operatorname{tr}_{\mathbb{C}^n}|A(x,\xi)|, \tag{4.106}$$

for matrix-valued functions A on $\partial\Lambda\times\partial\Gamma$, we estimate the right-hand side of (4.105) from above by

$$\begin{aligned}(m-1)\|A_1\|_{\infty,1}^m + (m-1)\|A_2\|_{\infty,1}^m + \sum_{k=1}^{m-1}\binom{m}{k}\|A_1\|_{\infty,1}^k\|A_2\|_{\infty,1}^{m-k}&\\ \leqslant (m-1)\big(\|A_1\|_{\infty,1}+\|A_2\|_{\infty,1}\big)^m&.\end{aligned}$$

Therefore, we conclude from the power-series expansion (4.70) of g that

$$\begin{aligned}\sup_{(x,\xi)\in\partial\Lambda\times\partial\Gamma}\big|\mathfrak{U}(g;A_1,A_2)\big| &\leqslant \sup_{(x,\xi)\in\partial\Lambda\times\partial\Gamma}\sum_{m=2}^\infty|\omega_m|\,\big|\mathfrak{U}(g_m;A_1,A_2)\big|\\ &\leqslant \frac{1}{(2\pi)^2}\sum_{m=2}^\infty|\omega_m|(m-1)t_0^m = \frac{t_0}{(2\pi)^2}\,g^{|1|}(t_0),\end{aligned} \tag{4.107}$$

where we used that $\|A_1\|_{\infty,1}+\|A_2\|_{\infty,1}\leqslant t_{A_1}+t_{A_2}\leqslant t_0$ by (4.75) and the definition of $g^{|1|}$ in (4.86). □

We are now ready to close the asymptotics.

Theorem 4.14. *Let $A_1,A_2\in C_b^\infty(\mathbb{R}^d\times\mathbb{R}^d,\mathbb{C}^{n\times n})$ be matrix-valued symbols with A_2 being compactly supported in the second variable. Let Λ be a bounded piece-wise C^1-admissible domain and Γ be a bounded piece-wise C^3-admissible domain. Let the function h be analytic in a disc of radius $R>t_0$*

with $h(0) = 0$*, then*

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(D_L(A_1,A_2;\Lambda,\Gamma)\big)\big] = L^d\Big(&\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(A_1)];\Lambda,\Gamma\big)+\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(A_2)];\Lambda,\Gamma^c\big)\Big)\\ &+L^{d-1}\log L\ \mathfrak{W}_1\big(\mathfrak{U}(h;A_1,A_2);\partial\Lambda,\partial\Gamma\big)\\ &+o(L^{d-1}\log L),\end{aligned}\tag{4.108}$$

as $L\to\infty$*. Here,* t_0 *was defined in* (4.77) *and* (4.75)*, the coefficients* $\mathfrak{W}_0$ *and* $\mathfrak{W}_1$ *in* (2.15) *and* (2.16)*, respectively, and the symbol* $\mathfrak{U}$ *in* (2.32)*.*

Proof. Let $p\in\mathbb{N}$ and approximate h by a polynomial in the following way

$$h=f_p+h_p,\quad f_p(z):=\sum_{m=1}^{p}\omega_m z^m,\qquad h_p(z):=h(z)-f_p(z)=\sum_{m=p+1}^{\infty}\omega_m z^m,\tag{4.109}$$

where $\omega_m:=h^{(m)}(0)/m!$ for $m\in\mathbb{N}$. Let $\varepsilon>0$. Then one can choose $p\in\mathbb{N}$ such that $h_p^{|1|}(t_0)<\frac{\varepsilon}{2}$. Lemma 4.12 applied to h_p yields

$$\big\|h_p\big(D_L(A_1,A_2)\big)-D_L\big(h_p(A_1),h_p(A_2)\big)\big\|_1\leqslant C_1\frac{\varepsilon}{2}L^{d-1}\log L+C_2L^{d-1}.\tag{4.110}$$

As

$$\begin{aligned}&\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(D_L(A_1,A_2)\big)-D_L\big(h(A_1),h(A_2)\big)\big]\\ &\qquad\leqslant\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[f_p\big(D_L(A_1,A_2)\big)-D_L\big(f_p(A_1),f_p(A_2)\big)\big]\\ &\qquad\quad+\big\|h_p\big(D_L(A_1,A_2)\big)-D_L\big(h_p(A_1),h_p(A_2)\big)\big\|_1,\end{aligned}\tag{4.111}$$

and the asymptotic formula is already established for f_p, we have

$$\limsup_{L\to\infty}\frac{\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(D_L(A_1,A_2)\big)-D_L\big(h(A_1),h(A_2)\big)\big]}{L^{d-1}\log L}\leqslant\mathfrak{W}_1(f_p)+C_1\frac{\varepsilon}{2},\tag{4.112}$$

where $\mathfrak{W}_1(f_p):=\mathfrak{W}_1\big(\mathfrak{U}(f_p;A_1,A_2);\partial\Lambda,\partial\Gamma\big)$. For the coefficient $\mathfrak{W}_1(h_p)$, Lemma 4.13 yields

$$|\mathfrak{W}_1(h_p)|\leqslant Ch_p^{|1|}(t_0)<C\frac{\varepsilon}{2}.\tag{4.113}$$

Hence

$$\mathfrak{W}_1(f_p)\leqslant\mathfrak{W}_1(h)+|\mathfrak{W}_1(h_p)|<\mathfrak{W}_1(h)+C\frac{\varepsilon}{2}.\tag{4.114}$$

Therefore, we have

$$\limsup_{L\to\infty}\frac{\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(D_L(A_1,A_2)\big)-D_L\big(h(A_1),h(A_2)\big)\big]}{L^{d-1}\log L}\leqslant\mathfrak{W}_1(h)+C\varepsilon.\tag{4.115}$$

The corresponding lower bound for the liminf is found in the same way. As ε is arbitrary, we obtain

$$\lim_{L\to\infty}\frac{\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(D_L(A_1,A_2)\big)-D_L\big(h(A_1),h(A_2)\big)\big]}{L^{d-1}\log L}=\mathfrak{W}_1(h).\tag{4.116}$$

The trace of $D_L(h(A_1),h(A_2))$ gives rise to the volume terms by Lemma 4.8, and we obtain the desired asymptotics

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(D_L(A_1,A_2;\Lambda,\Gamma)\big)\big] = L^d\Big(&\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(A_1)];\Lambda,\Gamma\big)+\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(A_2)];\Lambda,\Gamma^c\big)\Big)\\ &+L^{d-1}\log L\ \mathfrak{W}_1\big(\mathfrak{U}(h;A_1,A_2);\partial\Lambda,\partial\Gamma\big)\\ &+o(L^{d-1}\log L),\end{aligned}\tag{4.117}$$

as $L\to\infty$. □

4.5. Closing the asymptotics: Smooth functions

We continue with arbitrarily often differentiable functions g vanishing at zero. In order to apply g to an operator, we restrict ourselves to the self-adjoint operator G_L, see (2.31) for the definition.

The trace of $D_L\big(g(\operatorname{Re} A_1), g(\operatorname{Re} A_2)\big)$ can again be computed explicitly and coincides, up to area terms, with the expected volume term. This is stated as

Lemma 4.15. *Let $A_1, A_2 \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be matrix-valued symbols with A_2 being compactly supported in the second variable. Further, let Λ and Γ be bounded admissible domains. Then, for any function $g \in C^\infty(\mathbb{R})$ with $g(0) = 0$, we have*

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} &\Big[D_L\big(g(\operatorname{Re} A_1), g(\operatorname{Re} A_2)\big)\Big] \\ &= L^d\Big[\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[g(\operatorname{Re} A_1)];\Lambda,\Gamma\big) + \mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[g(\operatorname{Re} A_2)];\Lambda,\Gamma^c\big)\Big] + O(L^{d-1}), \quad (4.118)\end{aligned}$$

as $L \to \infty$.

Proof. Let $\phi, \psi \in C_c^\infty(\mathbb{R}^d)$ be as in (4.37), i.e. $\phi|_\Lambda = 1$ and $\psi|_\Gamma = 1$. First note that the function g being smooth guarantees that $g(\operatorname{Re} A_j) \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ is a well-defined symbol for $j \in \{1,2\}$. Further, the property $g(0) = 0$ ensures that these symbols are again compactly supported whenever the corresponding symbol A_j is compactly supported. Therefore, the previous results (4.40) and (4.41) on C_b^∞-symbols apply and we obtain

$$\begin{aligned}D_L\big(g(\operatorname{Re} A_1), g(\operatorname{Re} A_2)\big) \sim\ &\mathbf{1}_\Lambda \operatorname{Op}_L^l\big(g(\operatorname{Re} A_1)\phi\psi\big)\operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda \\ &+ \mathbf{1}_\Lambda \operatorname{Op}_L^l\big(g(\operatorname{Re} A_2)\phi\big)\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Lambda. \quad (4.119)\end{aligned}$$

The trace of the right-hand side can be computed explicitly by integrating its kernel along the diagonal which yields

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} &\big[\mathbf{1}_\Lambda \operatorname{Op}_L^l\big(g(\operatorname{Re} A_1)\phi\psi\big)\operatorname{Op}_L(\mathbf{1}_\Gamma)\mathbf{1}_\Lambda + \mathbf{1}_\Lambda \operatorname{Op}_L^l\big(g(\operatorname{Re} A_2)\phi\big)\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Lambda\big] \\ &= L^d\Big[\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[g(\operatorname{Re} A_1)];\Lambda,\Gamma\big) + \mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[g(\operatorname{Re} A_2)];\Lambda,\Gamma^c\big)\Big]. \quad (4.120)\end{aligned}$$

□

We continue by estimating the trace norm

$$\big\|g\big(G_L(A_1, A_2)\big) - D_L\big(g(\operatorname{Re} A_1), g(\operatorname{Re} A_2)\big)\big\|_1. \quad (4.121)$$

The line of argumentation is similar to the analytic case, where each ingredient is replaced by a counterpart for smooth functions.

Lemma 4.16. *Let $A_1, A_2 \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be matrix-valued symbols with A_2 being compactly supported in the second variable. Further, let Λ and Γ be bounded admissible domains. Then there exist symbols $B_1, B_2 \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ which are compactly supported in both variables and with $(A_1 - B_1)|_{\Lambda\times\Gamma} = 0$, $(A_2 - B_2)|_{\Lambda\times\mathbb{R}^d} = 0$, such that for any smooth function $g \in C_c^\infty(\mathbb{R})$ with $g(0) = 0$ we have*

$$D_L\big(g(\operatorname{Re} A_1), g(\operatorname{Re} A_2)\big) \sim D_L\big(g(\operatorname{Re} B_1), g(\operatorname{Re} B_2)\big) \quad (4.122)$$

and

$$g\big(G_L(A_1, A_2)\big) \sim g\big(G_L(B_1, B_2)\big). \quad (4.123)$$

Proof. Let $L \geqslant 1$. We find the compactly supported symbols by introducing smooth cut-off functions in the same way as in the proof of Lemma 4.9: Let $\phi, \psi \in C_c^\infty(\mathbb{R}^d)$ be as in (4.37) and define $B_1 := A_1\phi\psi$ and $B_2 := A_2\phi$.

We note that in the proof of (4.78) it was sufficient that $g(A_j), g(B_j) \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ are well-defined symbols for $j \in \{1,2\}$, which are compactly supported whenever the respective symbols A_j, B_j are compactly supported. For the Hermitian matrix-valued symbols $\operatorname{Re} A_j, \operatorname{Re} B_j$ this is the case if g is smooth with $g(0) = 0$. Therefore, we have

$$D_L\big(g(\operatorname{Re} A_1), g(\operatorname{Re} A_2)\big) \sim D_L\big(g(\operatorname{Re} B_1), g(\operatorname{Re} B_2)\big). \tag{4.124}$$

This proves (4.122), even without the requirement that g is compactly supported.

In order to prove (4.123), we apply (4.122) with $g = 1$, i.e.

$$D_L(\operatorname{Re} A_1, \operatorname{Re} A_2) \sim D_L(\operatorname{Re} B_1, \operatorname{Re} B_2). \tag{4.125}$$

Using (4.58) on both sides, this extends to

$$G_L\big(A_1, A_2\big) \sim G_L\big(B_1, B_2\big). \tag{4.126}$$

We write

$$g\big(G_L(A_1,A_2)\big) - g\big(G_L(B_1,B_2)\big) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \Big(\mathrm{e}^{\mathrm{i}tG_L(A_1,A_2)} - \mathrm{e}^{\mathrm{i}tG_L(B_1,B_2)}\Big)\, \hat{g}(t)\,\mathrm{d}t, \tag{4.127}$$

where $\hat{g} \in \mathcal{S}(\mathbb{R})$ is the Fourier transform of g. The operator $E(t) := \mathrm{e}^{\mathrm{i}tG_L(A_1,A_2)} - \mathrm{e}^{\mathrm{i}tG_L(B_1,B_2)}$ satisfies the following differential equation

$$\mathrm{i}\partial_t E(t) + G_L(A_1,A_2)E(t) = -\big(G_L(A_1,A_2) - G_L(B_1,B_2)\big)\,\mathrm{e}^{\mathrm{i}tG_L(B_1,B_2)} =: M(t). \tag{4.128}$$

As $E(0) = 0$, we obtain

$$E(t) = -\mathrm{i}\int_0^t \mathrm{e}^{\mathrm{i}(t-s)G_L(A_1,A_2)}\, M(s)\,\mathrm{d}s. \tag{4.129}$$

As $G_L(B_1,B_2)$ is self-adjoint, we have

$$\|M(t)\|_1 \leqslant \|G_L(A_1,A_2) - G_L(B_1,B_2)\|_1 \leqslant CL^{d-1}, \tag{4.130}$$

where C is independent of t. The operator $G_L(A_1,A_2)$ is also self-adjoint. Therefore,

$$\|E(t)\|_1 \leqslant CL^{d-1}t. \tag{4.131}$$

By (4.127) we conclude that

$$\big\|g\big(G_L(A_1,A_2)\big) - g\big(G_L(B_1,B_2)\big)\big\|_1 \leqslant CL^{d-1}. \tag{4.132}$$

□

Next, we quote a special case of [Sob17, Cor. 2.11] adapted to our situation.

Lemma 4.17. *Let $g \in C_c^2(\mathbb{R})$ and $q \in\,]0,1[$. Let X be a self-adjoint operator on a dense domain $\mathcal{D}$ in a separable Hilbert space $\mathcal{H}$ and P be an orthogonal projection on $\mathcal{H}$ such that $P\mathcal{D} \subseteq \mathcal{D}$ and $PX(1_{\mathcal{H}} - P) \in \mathcal{T}_q$. Then there exists a constant $C > 0$, independent of X, P and g, such that*

$$\|g(PXP)P - Pg(X)\|_1 \leqslant C \max_{0\leqslant k\leqslant 2} \|g^{(k)}\|_\infty \|PX(1_{\mathcal{H}} - P)\|_q^q. \tag{4.133}$$

We continue with the commutation of the test function g with the left-operator. Here, the matrix nature of the symbol leads to some additional difficulties. We first define, for a given matrix-valued symbol $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ and a smooth function $g \in C_c^\infty(\mathbb{R})$, the matrix-valued amplitude $A_g \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$, given by

$$A_g(x, y, \xi) := g\Big(\tfrac{1}{2}\big(\operatorname{Re} A(x, \xi) + \operatorname{Re} A(y, \xi)\big)\Big) \tag{4.134}$$

for $x, y, \xi \in \mathbb{R}^d$. As a preparatory result we first derive bounds for the symbol norm of an exponential of A_{id} the amplitude (4.134) for the functions $g = 1$.

Lemma 4.18. *Let $A \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be a matrix-valued symbol with compact support in both variables. Let $m_x, m_y, m_\xi \in \mathbb{N}_0$. Then there exist constants $C_1, C_2 > 0$, independent of t, such that*

$$\mathbf{N}^{(m_x,m_y,m_\xi)}(\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}}) \leqslant Ct^{(m_x+m_y+m_\xi)} \tag{4.135}$$

and

$$\mathbf{N}^{(m_x,m_\xi)}(\mathrm{e}^{\mathrm{i}t\operatorname{Re} A}) \leqslant Ct^{(m_x+m_\xi)}. \tag{4.136}$$

The symbol norm $\mathbf{N}$ is defined in Definition 2.8.

Proof. We begin by stating a version of Duhamel's formula adapted to our situation. Let $B \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be a matrix-valued amplitude and let s be any of the Cartesian components of x, y, ξ. We consider the $C^\infty(\mathbb{R}, \mathbb{C}^{n\times n})$ map given by $s \mapsto B(s)$ with the other coordinates being fixed. Then Duhamel's formula reads

$$\frac{\mathrm{d}}{\mathrm{d}s}\,\mathrm{e}^{B(s)} = \int_0^1 \mathrm{e}^{\sigma B(s)}\,\frac{\mathrm{d}B}{\mathrm{d}s}\,\mathrm{e}^{(1-\sigma)B(s)}\,\mathrm{d}\sigma. \tag{4.137}$$

For the reader's convenience and as it is not easy to find in the literature, we also give a proof of (4.137). Let $j \in \{1, \dots, d\}$, we focus on the case $s = x_j$, i.e. we show

$$\frac{\partial}{\partial x_j}\,\mathrm{e}^{B(x,y,\xi)} = \int_0^1 \mathrm{e}^{\sigma B(x,y,\xi)}\,\frac{\partial B}{\partial x_j}(x, y, \xi)\,\mathrm{e}^{(1-\sigma)B(x,y,\xi)}\,\mathrm{d}\sigma \tag{4.138}$$

for every $x, y, \xi \in \mathbb{R}^d$. The other cases work in the same way. For $h \neq 0$, we consider the expression

$$E(\sigma) := \mathrm{e}^{\sigma B(x+he_j,y,\xi)}\,\mathrm{e}^{(1-\sigma)B(x,y,\xi)} \tag{4.139}$$

which is continuously differentiable in σ and write

$$\mathrm{e}^{B(x+he_j,y,\xi)} - \mathrm{e}^{B(x,y,\xi)} = E(1) - E(0) = \int_0^1 \frac{\mathrm{d}E}{\mathrm{d}\sigma}\,\mathrm{d}\sigma. \tag{4.140}$$

Expanding the exponential function in a power series, we see that $\frac{\mathrm{d}\,\mathrm{e}^{\sigma C}}{\mathrm{d}\sigma} = C\,\mathrm{e}^{\sigma C} = \mathrm{e}^{\sigma C}\,C$ for the square matrices $C \in \{B(x + he_j, y, \xi), B(x, y, \xi)\}$. Hence, the right-hand side of (4.140) is equal to

$$\int_0^1 \mathrm{e}^{\sigma B(x+he_j,y,\xi)}\,[B(x + he_j, y, \xi) - B(x, y, \xi)]\,\mathrm{e}^{(1-\sigma)B(x,y,\xi)}\,\mathrm{d}\sigma \tag{4.141}$$

and therefore

$$\tfrac{1}{h}\big[\,\mathrm{e}^{B(x+he_j,y,\xi)} - \mathrm{e}^{B(x,y,\xi)}\,\big] = \int_0^1 \mathrm{e}^{\sigma B(x+he_j,y,\xi)}\,\tfrac{1}{h}[B(x+he_j, y, \xi) - B(x, y, \xi)]\,\mathrm{e}^{(1-\sigma)B(x,y,\xi)}\,\mathrm{d}\sigma \tag{4.142}$$

Expanding the matrix-valued amplitude in each entry with Taylor's theorem

$$B(x + he_j, y, \xi) - B(x, y, \xi) = h\frac{\partial B}{\partial x_j}(x, y, \xi) + h^2\int_0^1 (1 - t)\frac{\partial^2 B}{\partial x_j^2}(x + hte_j, y, \xi)\,\mathrm{d}t \tag{4.143}$$

and taking the limit $h \to 0$ in (4.142) proves Duhamel's formula (4.137).

With this at hand, we are ready to prove (4.135). Let s_1 be any of the Cartesian components of either x, y or ξ. Then, by (4.137), we have

$$\begin{aligned}\sup_{x,y,\xi\in\mathbb{R}^d} \operatorname{tr}_{\mathbb{C}^n}& \left|\frac{\partial}{\partial s_1} \mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}(x,y,\xi)}\right| \\ &= \sup_{x,y,\xi\in\mathbb{R}^d} \operatorname{tr}_{\mathbb{C}^n}\left|\int_0^1 \mathrm{e}^{\sigma\mathrm{i}tA_{\mathrm{id}}(x,y,\xi)} \frac{\partial}{\partial s_1}\mathrm{i}tA_{\mathrm{id}}(x,y,\xi)\,\mathrm{e}^{(1-\sigma)\mathrm{i}tA_{\mathrm{id}}(x,y,\xi)}\,\mathrm{d}\sigma\right| \\ &\leqslant t\,\mathbf{N}^{(m_x,m_y,m_\xi)}(A_{\mathrm{id}}),\end{aligned} \tag{4.144}$$

where we used that $A_{\mathrm{id}}(x,y,\xi)$ is unitary. As the bound on the right-hand side of (4.144) is independent of the choice of s_1, (4.135) follows in the case $m_x+m_y+m_\xi=1$. If now s_2 is a second Cartesian component, (4.137) yields

$$\frac{\partial^2}{\partial s_2\partial s_1}\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}} = \frac{\partial}{\partial s_2}\int_0^1 \mathrm{e}^{\sigma\mathrm{i}tA_{\mathrm{id}}}\frac{\partial}{\partial s_1}\mathrm{i}tA_{\mathrm{id}}\,\mathrm{e}^{(1-\sigma)\mathrm{i}tA_{\mathrm{id}}}\,\mathrm{d}\sigma. \tag{4.145}$$

As the integrand on the right-hand side is still smooth in s_2, the right-hand side is equal to

$$\begin{aligned}&-t^2\int_0^1\int_0^1 \mathrm{e}^{\sigma\sigma'\mathrm{i}tA_{\mathrm{id}}}\frac{\partial A_{\mathrm{id}}}{\partial s_2}\mathrm{e}^{\sigma(1-\sigma')\mathrm{i}tA_{\mathrm{id}}}\frac{\partial A_{\mathrm{id}}}{\partial s_1}\mathrm{e}^{(1-\sigma)\mathrm{i}tA_{\mathrm{id}}}\,\mathrm{d}\sigma'\,\mathrm{d}\sigma \\ &+\mathrm{i}t\int_0^1 \mathrm{e}^{\sigma\mathrm{i}tA_{\mathrm{id}}}\frac{\partial^2 A_{\mathrm{id}}}{\partial s_2 s_1}\mathrm{e}^{(1-\sigma)\mathrm{i}tA_{\mathrm{id}}}\,\mathrm{d}\sigma \\ &-t^2\int_0^1\int_0^1 \mathrm{e}^{\sigma\mathrm{i}tA_{\mathrm{id}}}\frac{\partial A_{\mathrm{id}}}{\partial s_1}\mathrm{e}^{(1-\sigma)\sigma'\mathrm{i}tA_{\mathrm{id}}}\frac{\partial A_{\mathrm{id}}}{\partial s_2}\mathrm{e}^{(1-\sigma)(1-\sigma')\mathrm{i}tA_{\mathrm{id}}}\,\mathrm{d}\sigma'\,\mathrm{d}\sigma,\end{aligned} \tag{4.146}$$

by the product rule. This entails the bound

$$\sup_{x,y,\xi\in\mathbb{R}^d}\operatorname{tr}_{\mathbb{C}^n}\left|\frac{\partial^2}{\partial s_2\partial s_1}\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}(x,y,\xi)}\right| \leqslant 3t^2\left(\mathbf{N}^{(m_x,m_y,m_\xi)}(A_{\mathrm{id}})\right)^2 \tag{4.147}$$

and proves (4.135) in the case $m_x+m_y+m_\xi=2$. Iteration of this procedure yields (4.135) for arbitrary $m_x, m_y, m_\xi \in \mathbb{N}_0$.

The proof of (4.136) works in the same way. □

We are now ready to prove the commutation of the smooth function g with the left-operator up to area terms.

Lemma 4.19. *Let $A \in C_b^\infty(\mathbb{R}^d\times\mathbb{R}^d, \mathbb{C}^{n\times n})$ be a matrix-valued symbol with compact support in both variables and let $g \in C_c^\infty(\mathbb{R})$ be a smooth function with compact support such that $g(0)=0$. Then we have*

$$g\big(\operatorname{Re}\operatorname{Op}_L^l(\operatorname{Re}A)\big) \sim \operatorname{Op}_L^{lr}(A_g) \sim \operatorname{Op}_L^l\left(g(\operatorname{Re}A)\right). \tag{4.148}$$

Proof. Let $L \geqslant 1$. First note that $\operatorname{Re}\operatorname{Op}_L^l(\operatorname{Re}A) = \operatorname{Op}_L^{lr}(A_{\mathrm{id}})$. Using linearity, we write

$$g\big(\operatorname{Op}_L^{lr}(A_{\mathrm{id}})\big) - \operatorname{Op}_L^{lr}(A_g) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\left(\mathrm{e}^{\mathrm{i}t\operatorname{Op}_L^{lr}(A_{\mathrm{id}})} - \operatorname{Op}_L^{lr}(\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}})\right)\hat{g}(t)\,\mathrm{d}t, \tag{4.149}$$

where $\hat{g}\in\mathcal{S}(\mathbb{R})$ is again the Fourier transform of g. The operator $E(t) := \operatorname{Op}_L^{lr}(\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}}) - \mathrm{e}^{\mathrm{i}t\operatorname{Op}_L^{lr}(A_{\mathrm{id}})}$ satisfies the following differential equation

$$\mathrm{i}\partial_t E(t) + \operatorname{Op}_L^{lr}(A_{\mathrm{id}})E(t) = \operatorname{Op}_L^{lr}(A_{\mathrm{id}})\operatorname{Op}_L^{lr}(\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}}) - \operatorname{Op}_L^{lr}(A_{\mathrm{id}}\,\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}}) =: M(t). \tag{4.150}$$

As $E(0) = 0$, we obtain

$$E(t) = -\mathrm{i}\int_0^t \mathrm{e}^{\mathrm{i}(t-s)\operatorname{Op}_L^{lr}(A_{\mathrm{id}})} M(s)\,\mathrm{d}s. \tag{4.151}$$

The next goal is to estimate the trace norm of $M(t)$ for given $t \in \mathbb{R}$. The triangle inequality yields

$$\begin{aligned}\|M(t)\|_1 \leqslant {} & \big\|\operatorname{Op}_L^{lr}(A_{\mathrm{id}})\operatorname{Op}_L^{lr}(\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}}) - \operatorname{Op}_L^{lr}(A_{\mathrm{id}})\operatorname{Op}_L^{l}(\mathrm{e}^{\mathrm{i}t\operatorname{Re}A})\big\|_1 \\ & + \big\|\operatorname{Op}_L^{lr}(A_{\mathrm{id}})\operatorname{Op}_L^{l}(\mathrm{e}^{\mathrm{i}t\operatorname{Re}A}) - \operatorname{Op}_L^{l}(\operatorname{Re}A)\operatorname{Op}_L^{l}(\mathrm{e}^{\mathrm{i}t\operatorname{Re}A})\big\|_1 \\ & + \big\|\operatorname{Op}_L^{l}(\operatorname{Re}A)\operatorname{Op}_L^{l}(\mathrm{e}^{\mathrm{i}t\operatorname{Re}A}) - \operatorname{Op}_L^{l}(\operatorname{Re}A\,\mathrm{e}^{\mathrm{i}t\operatorname{Re}A})\big\|_1 \\ & + \big\|\operatorname{Op}_L^{l}(\operatorname{Re}A\,\mathrm{e}^{\mathrm{i}t\operatorname{Re}A}) - \operatorname{Op}_L^{lr}(A_{\mathrm{id}}\,\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}})\big\|_1.\end{aligned} \tag{4.152}$$

We will now estimate each of these trace norms individually. Let $\phi \in C_c^\infty(\mathbb{R}^d)$ be a function such that $\phi(x)A(x,\xi) = A(x,\xi)$ for all $x,\xi \in \mathbb{R}^d$. We decompose the amplitude $\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}}$ as

$$\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}(x,y,\xi)} = \mathbb{1}_n + \phi(x)\big(\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}(x,y,\xi)} - \mathbb{1}_n\big) + \big(1-\phi(x)\big)\big(\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}(x,y,\xi)} - \mathbb{1}_n\big), \tag{4.153}$$

where the second term is compactly supported in the variable x, and the third term is compactly supported in the variable y. To see the latter, we note that for all $x \in \mathbb{R}^d$ such that the function $\xi \mapsto \operatorname{Re}A(x,\xi)$ is not zero we have $(1-\phi(x)) = 0$ and therefore $\operatorname{Re}A(y,\xi) = 0$ implies that the third term on the right-hand side of (4.153) is already zero, independently of $x \in \mathbb{R}^d$. Similarly, we write

$$\mathrm{e}^{\mathrm{i}t\operatorname{Re}A(x,\xi)} = \mathbb{1}_n + \phi(x)\big(\mathrm{e}^{\mathrm{i}t\operatorname{Re}A(x,\xi)} - \mathbb{1}_n\big). \tag{4.154}$$

Therefore and since $\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}(x,x,\xi)} = \mathrm{e}^{\mathrm{i}t\operatorname{Re}A(x,\xi)}$ for all $x,\xi \in \mathbb{R}^d$, the estimate (3.21) is applicable and yields

$$\begin{aligned}&\big\|\operatorname{Op}_L^{lr}(\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}}) - \operatorname{Op}_L^{l}(\mathrm{e}^{\mathrm{i}t\operatorname{Re}A})\big\|_1 \\ &\leqslant \big\|\operatorname{Op}_L^{lr}\big(\phi(\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}} - \mathbb{1}_n)\big) - \operatorname{Op}_L^{l}\big(\phi(\mathrm{e}^{\mathrm{i}t\operatorname{Re}A} - \mathbb{1}_n)\big)\big\|_1 + \big\|\operatorname{Op}_L^{lr}\big((1-\phi)(\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}} - \mathbb{1}_n)\big)\big\|_1 \\ &\leqslant C_1L^{d-1}\Big(\mathbf{N}^{(d+1,d+1,d+2)}\big(\phi(\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}} - \mathbb{1}_n)\big) + \mathbf{N}^{(d+1,d+1,d+2)}\big((1-\phi)(\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}} - \mathbb{1}_n)\big)\Big).\end{aligned} \tag{4.155}$$

We note here, that we only need to control the dependence on L and t of the estimate. Therefore, we directly subsume the dependence on the support of the amplitude in (3.21) into the constant C_1. We will also do this in the following estimates.
Next, writing $A_{\mathrm{id}}(x,y,\xi) = \frac{1}{2}\operatorname{Re}A(x,\xi) + \frac{1}{2}\operatorname{Re}A(y,\xi)$, the estimate (3.22) yields

$$\big\|\operatorname{Op}_L^{lr}(A_{\mathrm{id}}) - \operatorname{Op}_L^{l}(\operatorname{Re}A)\big\|_1 = \tfrac{1}{2}\big\|\operatorname{Op}_L^{r}(\operatorname{Re}A) - \operatorname{Op}_L^{l}(\operatorname{Re}A)\big\|_1 \leqslant C_2L^{d-1}\mathbf{N}^{(d+1,d+2)}(\operatorname{Re}A). \tag{4.156}$$

As the symbol A is compactly supported in both variables, the estimate (3.29) yields

$$\begin{aligned}&\big\|\operatorname{Op}_L^{l}(\operatorname{Re}A)\operatorname{Op}_L^{l}(\mathrm{e}^{\mathrm{i}t\operatorname{Re}A}) - \operatorname{Op}_L^{l}(\operatorname{Re}A\,\mathrm{e}^{\mathrm{i}t\operatorname{Re}A})\big\|_1 \\ &\qquad\leqslant C_3L^{d-1}\mathbf{N}^{(d+1,d+2)}(\operatorname{Re}A)\,\mathbf{N}^{(d+1,d+2)}(\mathrm{e}^{\mathrm{i}t\operatorname{Re}A}).\end{aligned} \tag{4.157}$$

We define the amplitudes $A^{(1)}(x,y,\xi) := \operatorname{Re}A(x,\xi)\,\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}(x,y,\xi)}$ and $A^{(2)}(x,y,\xi) := \operatorname{Re}A(y,\xi)\,\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}(x,y,\xi)}$, which are compactly supported in the variables x, respectively y. With estimate (3.21) we obtain

$$\begin{aligned}&\big\|\operatorname{Op}_L^{l}(\operatorname{Re}A\,\mathrm{e}^{\mathrm{i}t\operatorname{Re}A}) - \operatorname{Op}_L^{lr}(A_{\mathrm{id}}\,\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}})\big\|_1 \\ &\leqslant \tfrac{1}{2}\big\|\operatorname{Op}_L^{l}(\operatorname{Re}A\,\mathrm{e}^{\mathrm{i}t\operatorname{Re}A}) - \operatorname{Op}_L^{lr}(A^{(1)})\big\|_1 + \tfrac{1}{2}\big\|\operatorname{Op}_L^{l}(\operatorname{Re}A\,\mathrm{e}^{\mathrm{i}t\operatorname{Re}A}) - \operatorname{Op}_L^{lr}(A^{(2)})\big\|_1 \\ &\leqslant C_4L^{d-1}\mathbf{N}^{(d+1,d+1,d+2)}(A^{(1)}).\end{aligned} \tag{4.158}$$

Combining the estimates (4.155) – (4.158), we obtain the following bound for the right-hand side of (4.152)

$$\begin{aligned} &C_1 L^{d-1} \| \operatorname{Op}_L^{lr}(A_{\mathrm{id}})\| \Big(\mathbf{N}^{(d+1,d+1,d+2)}\big(\phi(\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}} - \mathbb{1}_n)\big) + \mathbf{N}^{(d+1,d+1,d+2)}\big((1-\phi)(\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}} - \mathbb{1}_n)\big)\Big) \\ &\quad + C_2 L^{d-1} \| \operatorname{Op}_L^{l}(\mathrm{e}^{\mathrm{i}t\operatorname{Re}A})\| \, \mathbf{N}^{(d+1,d+2)}(\operatorname{Re}A) \\ &\quad + C_3 L^{d-1} \mathbf{N}^{(d+1,d+2)}(\operatorname{Re}A)\, \mathbf{N}^{(d+1,d+2)}(\mathrm{e}^{\mathrm{i}t\operatorname{Re}A}) \\ &\quad + C_4 L^{d-1} \mathbf{N}^{(d+1,d+1,d+2)}(A^{(1)}). \end{aligned} \tag{4.159}$$

In order to proceed, we apply Lemma 3.1 to bound $\| \operatorname{Op}_L^{lr}(A_{\mathrm{id}})\|$ uniformly in $L \geqslant 1$ and to estimate $\| \operatorname{Op}_L^{l}(\mathrm{e}^{\mathrm{i}t\operatorname{Re}A})\| \leqslant C\mathbf{N}^{(d,d+1)}(\mathrm{e}^{\mathrm{i}t\operatorname{Re}A})$. It remains to estimate the t-dependence of the symbol norms. Each differentiation of the matrix exponentials $\mathrm{e}^{\mathrm{i}tA_{\mathrm{id}}}(x,y,\xi)$, respectively $\mathrm{e}^{\mathrm{i}t\operatorname{Re}A}(x,\xi)$, with respect to the Cartesian components of x, y, ξ, respectively x, ξ, brings down a factor of t according to Lemma 4.18. Together with the unitarity of $A_{\mathrm{id}}(x,y,\xi)$ and $\operatorname{Re}A(x,\xi)$, we infer from (4.159) and (4.152) that

$$\|M(t)\|_1 \leqslant CL^{d-1} t^{(3d+4)}, \tag{4.160}$$

where the constant C is independent of L and t. As the operator $\operatorname{Op}_L^{lr}(A_{\mathrm{id}})$ is self-adjoint, we conclude from (4.151) that

$$\|E(t)\|_1 \leqslant CL^{d-1} t^{(3d+5)}. \tag{4.161}$$

By (4.149) we conclude that

$$g\big(\operatorname{Re}\operatorname{Op}_L^{l}(\operatorname{Re}A)\big) \sim \operatorname{Op}_L^{lr}(A_g). \tag{4.162}$$

With the same function ϕ as in (4.153), we write $A_g(x,y,\xi) = \phi(x)A_g(x,y,\xi) + \big(1-\phi(x)\big)A_g(x,y,\xi)$ and note that ϕA_g is compactly supported in the variable x and $(1-\phi)A_g$ is compactly supported in the variable y. Applying relation (3.15) from Lemma 3.5, yields

$$\begin{aligned} \operatorname{Op}_L^{lr}(A_g) &= \operatorname{Op}_L^{lr}(\phi A_g) + \operatorname{Op}_L^{lr}\big((1-\phi)A_g\big) \\ &\sim \operatorname{Op}_L^{l}\big(\phi g(\operatorname{Re}A)\big) + \operatorname{Op}_L^{l}\big((1-\phi)g(\operatorname{Re}A)\big) = \operatorname{Op}_L^{l}\big(g(\operatorname{Re}A)\big). \end{aligned} \tag{4.163}$$

□

We now combine the results for smooth functions in order to obtain the desired estimate for (4.121).

Lemma 4.20. *Let $A_1, A_2 \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be matrix-valued symbols with A_2 being compactly supported in the second variable. Further, let Λ and Γ be bounded admissible domains. For any function $g \in C_c^\infty(\mathbb{R})$ with $g(0) = 0$ there exist constants $C_1, C_2 > 0$, independent of L with C_1 also independent of g, such that*

$$\Big\|g\big(G_L(A_1,A_2)\big) - D_L\big(g(\operatorname{Re}A_1), g(\operatorname{Re}A_2)\big)\Big\|_1 \leqslant C_1 \max_{0\leqslant k\leqslant 2} \|g^{(k)}\|_\infty L^{d-1}\log L + C_2 L^{d-1} \tag{4.164}$$

for every $L \geqslant 2$.

Proof. The proof resembles the one of Lemma 4.12. Let $L \geqslant 2$. As Lemma 4.16 yields

$$g\big(G_L(A_1,A_2)\big) \sim g\big(G_L(B_1,B_2)\big) \tag{4.165}$$

and

$$D_L\big(g(\operatorname{Re}A_1), g(\operatorname{Re}A_2)\big) \sim D_L\big(g(\operatorname{Re}B_1), g(\operatorname{Re}B_2)\big), \tag{4.166}$$

it suffices to show (4.164) with A_1 and A_2 replaced by the compactly supported symbols B_1 and B_2.

Lemma 4.17 with $0 < q < 1$ applied to g, $\big(G_L(B_1, B_2; \mathbb{R}^d, \Gamma)\big)$ and $\mathbf{1}_\Lambda$, combined with Lemma 3.8, yields

$$\begin{aligned}
&\Big\| g\big(G_L(B_1, B_2)\big) - \mathbf{1}_\Lambda g\big(G_L(B_1, B_2; \mathbb{R}^d, \Gamma)\big)\mathbf{1}_\Lambda \Big\|_1 \\
&\qquad = \Big\| \big[g\big(G_L(B_1, B_2)\big)\mathbf{1}_\Lambda - \mathbf{1}_\Lambda g\big(G_L(B_1, B_2; \mathbb{R}^d, \Gamma)\big) \big] \mathbf{1}_\Lambda \Big\|_1 \\
&\qquad \leqslant C' \max_{0 \leqslant k \leqslant 2} \|g^{(k)}\|_\infty \Big(\|\mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} B_1) \operatorname{Op}_L(\mathbf{1}_\Gamma) \mathbf{1}_{\Lambda^c}\|_1 \\
&\qquad\qquad + \|\mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} B_2) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \mathbf{1}_{\Lambda^c}\|_1 \Big) \\
&\qquad \leqslant C_1 \max_{0 \leqslant k \leqslant 2} \|g^{(k)}\|_\infty L^{d-1} \log L. \qquad (4.167)
\end{aligned}$$

Here C' is the constant from Lemma 4.17, and C_1 is already the constant appearing in the claim in (4.164). For its independence of g and L we refer to Lemmas 4.17 and 3.8. In the first equality in (4.167) we used that $g(0) = 0$.

By an elementary property of the functional calculus we obtain

$$\begin{aligned}
g\big(G_L(B_1, B_2; \mathbb{R}^d, \Gamma)\big) &= g\big(\operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} B_1) \operatorname{Op}_L(\mathbf{1}_\Gamma)\big) \\
&\quad + g\big(\operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} B_2) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\big). \qquad (4.168)
\end{aligned}$$

Similarly to (4.167), we now apply Lemma 4.17 to $\operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} B_1)$ and $\operatorname{Op}_L(\mathbf{1}_\Gamma)$, followed by Lemma 3.8, which yields

$$\begin{aligned}
&\Big\| g\big(\operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} B_1) \operatorname{Op}_L(\mathbf{1}_\Gamma)\big) - \operatorname{Op}_L(\mathbf{1}_\Gamma) g\big(\operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} B_1)\big) \operatorname{Op}_L(\mathbf{1}_\Gamma) \Big\|_1 \\
&\qquad \leqslant C \max_{0 \leqslant k \leqslant 2} \|g^{(k)}\|_\infty \big\| \operatorname{Op}_L(\mathbf{1}_\Gamma) \operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} B_1) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \big\|_q^q \leqslant C L^{d-1}. \qquad (4.169)
\end{aligned}$$

Applying Lemma 4.17 again to $\operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} B_2)$ and $\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})$, we conclude

$$\begin{aligned}
\mathbf{1}_\Lambda g\big(G_L(B_1, B_2; \mathbb{R}^d, \Gamma)\big)\mathbf{1}_\Lambda &\sim \mathbf{1}_\Lambda \Big(\operatorname{Op}_L(\mathbf{1}_\Gamma) g\big(\operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} B_1)\big) \operatorname{Op}_L(\mathbf{1}_\Gamma) \\
&\quad + \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) g\big(\operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} B_2)\big) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \Big) \mathbf{1}_\Lambda. \qquad (4.170)
\end{aligned}$$

Finally, Lemma 4.19 yields

$$\mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_\Gamma) g\big(\operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} B_1)\big) \operatorname{Op}_L(\mathbf{1}_\Gamma) \mathbf{1}_\Lambda \sim T_L(g(\operatorname{Re} B_1); \Lambda, \Gamma), \qquad (4.171)$$

as well as

$$\mathbf{1}_\Lambda \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) g\big(\operatorname{Re} \operatorname{Op}_L^l(\operatorname{Re} B_2)\big) \operatorname{Op}_L(\mathbf{1}_{\Gamma^c}) \mathbf{1}_\Lambda \sim T_L\big(g(\operatorname{Re} B_2); \Lambda, \Gamma^c\big), \qquad (4.172)$$

which concludes the proof, since

$$D_L\big(g(\operatorname{Re} B_1), g(\operatorname{Re} B_2); \Lambda, \Gamma\big) = T_L\big(g(\operatorname{Re} B_1); \Lambda, \Gamma\big) + T_L\big(g(\operatorname{Re} B_2); \Lambda, \Gamma^c\big). \qquad (4.173)$$

□

We continue with an estimate for the coefficient $\mathfrak{W}_1$

Lemma 4.21. *Let $A_1, A_2 \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n \times n})$ be Hermitian matrix-valued symbols. Let the function $g \in C^1(\mathbb{R})$ be continuously differentiable with $g(0) = 0$. Let $\partial\Lambda$ and $\partial\Gamma$ have finite $(d-1)$-dimensional surface measure induced by Lebesgue measure on $\mathbb{R}^d$. Then there exists a constant $C > 0$, which does not depend on g, such that*

$$\big| \mathfrak{W}_1\big(\mathfrak{U}(g; A_1, A_2); \partial\Lambda, \partial\Gamma\big) \big| \leqslant C \|g'\|_\infty. \qquad (4.174)$$

Proof. As the surface measure of $\partial\Lambda$ and $\partial\Gamma$ is finite, it suffices to show

$$\sup_{(x,\xi)\in\partial\Lambda\times\partial\Gamma} \left|\big(\mathfrak{U}(g;A_1,A_2)\big)(x,\xi)\right| \leqslant C\|g'\|_\infty. \tag{4.175}$$

We use the fact that $\frac{1}{t(1-t)} = \frac{1}{t} + \frac{1}{(1-t)}$ to work towards a pointwise estimate for the function

$$\begin{aligned}(2\pi)^2\mathfrak{U}(g;A_1,A_2) &= \int_0^1 \frac{\operatorname{tr}_{\mathbb{C}^n}\left[g\big(A_1t+A_2(1-t)\big) - g(A_1)t - g(A_2)(1-t)\right]}{t}\,\mathrm{d}t \\ &\quad + \int_0^1 \frac{\operatorname{tr}_{\mathbb{C}^n}\left[g\big(A_1t+A_2(1-t)\big) - g(A_1)t - g(A_2)(1-t)\right]}{1-t}\,\mathrm{d}t.\end{aligned} \tag{4.176}$$

For the first integral we write

$$\begin{aligned}&\int_0^1 \frac{\operatorname{tr}_{\mathbb{C}^n}\left[g\big(A_1t+A_2(1-t)\big) - g(A_1)t - g(A_2)(1-t)\right]}{t}\,\mathrm{d}t \\ &\qquad = \int_0^1 \frac{\operatorname{tr}_{\mathbb{C}^n}\left[g\big(A_1t+A_2(1-t)\big) - g(A_2)\right]}{t}\,\mathrm{d}t - \operatorname{tr}_{\mathbb{C}^n}\left[g(A_1)-g(A_2)\right].\end{aligned} \tag{4.177}$$

We now require an estimate for the difference $\operatorname{tr}_{\mathbb{C}^n}[g(M_1)-g(M_2)]$ for Hermitian matrices $M_1, M_2 \in \mathbb{C}^{n\times n}$ in terms of $\|g'\|_\infty$. As $g \in C^1(\mathbb{R})$, we estimate

$$\left|\operatorname{tr}_{\mathbb{C}^n}[g(M_1)-g(M_2)]\right| \leqslant \int_0^1 \left|\frac{\mathrm{d}}{\mathrm{d}t}\operatorname{tr}_{\mathbb{C}^n}\left[g\big(M_2+t(M_1-M_2)\big)\right]\right|\mathrm{d}t \leqslant \|g'\|_\infty \operatorname{tr}_{\mathbb{C}^n}|M_1-M_2|. \tag{4.178}$$

Noting that $A_1t + A_2(1-t) - A_2 = A_1t - A_2t$, an application of (4.178) yields

$$\operatorname{tr}_{\mathbb{C}^n}\left[g\big(A_1t+A_2(1-t)\big) - g(A_2)\right] \leqslant \|g'\|_\infty(\|A_1\|_{\infty,1} + \|A_2\|_{\infty,1})\,t, \tag{4.179}$$

where the norms are defined in (4.106). Using this, we estimate the last line of (4.177) by

$$\begin{aligned}&\|g'\|_\infty\big(\|A_1\|_{\infty,1}+\|A_2\|_{\infty,1}\big)\int_0^1 \frac{t}{t}\,\mathrm{d}t \;+\; \|g'\|_\infty\big(\|A_1\|_{\infty,1}+\|A_2\|_{\infty,1}\big) \\ &\qquad = 2\|g'\|_\infty\big(\|A_1\|_{\infty,1}+\|A_2\|_{\infty,1}\big).\end{aligned}$$

Similarly, we obtain for the second integral

$$\begin{aligned}&\int_0^1 \frac{\operatorname{tr}_{\mathbb{C}^n}\left[g\big(A_1t+A_2(1-t)\big) - g(A_1)t - g(A_2)(1-t)\right]}{1-t}\,\mathrm{d}t \\ &\quad = \int_0^1 \frac{\operatorname{tr}_{\mathbb{C}^n}\left[g\big(A_1t+A_2(1-t)\big) - g(A_1)\right]}{1-t}\,\mathrm{d}t + \operatorname{tr}_{\mathbb{C}^n}[g(A_1)-g(A_2)] \\ &\quad \leqslant 2\|g'\|_\infty\big(\|A_1\|_{\infty,1}+\|A_2\|_{\infty,1}\big).\end{aligned} \tag{4.180}$$

Therefore, we conclude that $\sup_{(x,\xi)\in\partial\Lambda\times\partial\Gamma}\left|\big(\mathfrak{U}(g;A_1,A_2)\big)(x,\xi)\right| \leqslant C\|g'\|_\infty$. □

With this, we are again ready to close the asymptotics.

Theorem 4.22. *Let $A_1, A_2 \in C_b^\infty(\mathbb{R}^d\times\mathbb{R}^d, \mathbb{C}^{n\times n})$ be matrix-valued symbols with A_2 being compactly supported in the second variable. Let Λ be a bounded piece-wise C^1-admissible domain and Γ be a* *bounded piece-wise C^3-admissible domain. Let the function $h \in C^\infty(\mathbb{R})$ be smooth with $h(0) = 0$, then*

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} &\big[h\big(G_L(A_1, A_2; \Lambda, \Gamma)\big)\big] \\ &= L^d\Big[\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(\operatorname{Re} A_1)]; \Lambda, \Gamma\big) + \mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(\operatorname{Re} A_2)]; \Lambda, \Gamma^c\big)\Big] \\ &\quad + L^{d-1}\log L\ \mathfrak{W}_1\big(\mathfrak{U}(h; \operatorname{Re} A_1, \operatorname{Re} A_2); \partial\Lambda, \partial\Gamma\big) \\ &\quad + o(L^{d-1}\log L), \end{aligned} \tag{4.181}$$

as $L \to \infty$. Here, the coefficients $\mathfrak{W}_0$ and $\mathfrak{W}_1$ were defined in (2.15) *and* (2.16)*, respectively, and the symbol $\mathfrak{U}$ in* (2.32)*.*

Proof. As the operator $G_L(A_1, A_2; \Lambda, \Gamma)$ is bounded, we can assume that there exists a radius $t_0 > 1$ such that h is compactly supported in the closed interval $[-t_0, t_0]$. As $h \in C^\infty(\mathbb{R}) \subset C^2(\mathbb{R})$ with $h(0) = 0$, we write the function h as

$$h(t) = h'(0)\,t + \int_0^t \int_0^s h^{(2)}(\tau)\,\mathrm{d}\tau\,\mathrm{d}s, \qquad t \in \mathbb{R}, \tag{4.182}$$

where h' denotes the first and $h^{(2)}$ denotes the second derivative of h. Let $\varepsilon > 0$ be arbitrary. By the Theorem of Stone–Weierstrass we can find a polynomial p_ε defined on $[-t_0, t_0]$ such that the following bound holds

$$\max_{|t|\leqslant t_0} |h^{(2)}(t) - p_\varepsilon(t)| < \frac{\varepsilon}{8t_0^2}. \tag{4.183}$$

Defining the polynomial g_ε by $g_\varepsilon(t) := h'(0)t + \int_0^t\int_0^s p_\varepsilon(\tau)\,\mathrm{d}\tau\,\mathrm{d}s$ for all $t \in [-t_0, t_0]$, we obtain the following bound for the function $h_\varepsilon := h - g_\varepsilon$

$$\max_{0\leqslant k\leqslant 2}\max_{|t|\leqslant t_0} |h_\varepsilon^{(k)}(t)| < \frac{\varepsilon}{2}. \tag{4.184}$$

Applying Lemma 4.20 yields

$$\big\|h_\varepsilon\big(G_L(A_1, A_2)\big) - D_L\big(h_\varepsilon(\operatorname{Re} A_1), h_\varepsilon(\operatorname{Re} A_2)\big)\big\|_1 \leqslant C_1\frac{\varepsilon}{2}L^{d-1}\log L + C_2L^{d-1}. \tag{4.185}$$

As

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} &\big[h\big(G_L(A_1, A_2)\big) - D_L\big(h(\operatorname{Re} A_1), h(\operatorname{Re} A_2)\big)\big] \\ &\leqslant \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[g_\varepsilon\big(G_L(A_1, A_2)\big) - D_L\big(g_\varepsilon(\operatorname{Re} A_1), g_\varepsilon(\operatorname{Re} A_2)\big)\big] \\ &\quad + \big\|h_\varepsilon\big(G_L(A_1, A_2)\big) - D_L\big(h_\varepsilon(\operatorname{Re} A_1), h_\varepsilon(\operatorname{Re} A_2)\big)\big\|_1, \end{aligned} \tag{4.186}$$

and the asymptotic formula is already established for g_ε, we obtain

$$\limsup_{L\to\infty}\frac{\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(G_L(A_1, A_2)\big) - D_L\big(h(\operatorname{Re} A_1), h(\operatorname{Re} A_2)\big)\big]}{L^{d-1}\log L} \leqslant \mathfrak{W}_1(g_\varepsilon) + C_1\frac{\varepsilon}{2}, \tag{4.187}$$

where $\mathfrak{W}_1(g_\varepsilon) := \mathfrak{W}_1\big(\mathfrak{U}(g_\varepsilon; \operatorname{Re} A_1, \operatorname{Re} A_2); \partial\Lambda, \partial\Gamma\big)$. Lemma 4.21 yields

$$|\mathfrak{W}_1(h_\varepsilon)| < C\frac{\varepsilon}{2}. \tag{4.188}$$

Hence, we have

$$\mathfrak{W}_1(g_\varepsilon) \leqslant \mathfrak{W}_1(h) + |\mathfrak{W}_1(h_\varepsilon)| < \mathfrak{W}_1(h) + C\frac{\varepsilon}{2}. \tag{4.189}$$

Therefore,

$$\limsup_{L\to\infty} \frac{\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[h\big(G_L(A_1,A_2)\big) - D_L\big(h(\operatorname{Re}A_1), h(\operatorname{Re}A_2)\big)\right]}{L^{d-1}\log L} \leqslant \mathfrak{W}_1(h) + C\varepsilon. \tag{4.190}$$

The corresponding lower bound for the liminf is found in the same way. As ε is arbitrary, we obtain

$$\lim_{L\to\infty} \frac{\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[h\big(G_L(A_1,A_2)\big) - D_L\big(h(\operatorname{Re}A_1), h(\operatorname{Re}A_2)\big)\right]}{L^{d-1}\log L} = \mathfrak{W}_1(h). \tag{4.191}$$

The trace of $D_L\big(h(\operatorname{Re}A_1), h(\operatorname{Re}A_2)\big)$ gives rise to the volume terms by Lemma 4.15, and we obtain the desired asymptotic expansion

$$\begin{aligned}
&\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[h\big(G_L(A_1,A_2;\Lambda,\Gamma)\big)\right] \\
&\qquad = L^d\left[\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(\operatorname{Re}A_1)];\Lambda,\Gamma\big) + \mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(\operatorname{Re}A_2)];\Lambda,\Gamma^c\big)\right] \\
&\qquad\quad + L^{d-1}\log L\ \mathfrak{W}_1\big(\mathfrak{U}(h;\operatorname{Re}A_1,\operatorname{Re}A_2);\partial\Lambda,\partial\Gamma\big) \\
&\qquad\quad + o(L^{d-1}\log L),
\end{aligned} \tag{4.192}$$

as $L\to\infty$. □

4.6. Closing the asymptotics: More general functions

We now consider more general functions satisfying Assumption 2.5. For the readers convenience we recall this assumption here.

Assumption 4.23. Let $\gamma\in\,]0,1]$ and let $\mathcal{X} := \{x_1,x_2,\dots,x_N\}\subset\mathbb{R}, N\in\mathbb{N}$, be a finite collection of different points on the real line. Let $U_j\subset\mathbb{R}$, $j\in\{1,\dots,N\}$, be pairwise disjoint neighbourhoods of the points $x_j\in\mathcal{X}$. Given a function $h\in C(\mathbb{R})\cap C^2(\mathbb{R}\setminus\mathcal{X})$, we assume the existence of a constant $C>0$ such that for every $k\in\{0,1,2\}$ the estimate

$$\left|\frac{\mathrm{d}^k}{\mathrm{d}x^k}\big[h-h(x_j)\big](x)\right| \leqslant C|x-x_j|^{\gamma-k}, \tag{4.193}$$

holds for every $x\in U_j\setminus\{x_j\}$ and every $j\in\{1,\dots,N\}$. In particular, this implies that h is Hölder continuous at the points of $\mathcal{X}$.

As Lemma 4.19 is not available for C_c^2-functions, we will restrict ourselves to the case that the symbols A_1 and A_2 only depend on the variable ξ from now on.

In Lemma 4.26 and the proof of Theorem 4.29, which is the main result of this section, we will decompose $h = h_1 + h_2$, where $h_1\in C^2(\mathbb{R})$ and h_2 is a finite sum of functions of the following type.

Assumption 4.24. Let $\gamma\in\,]0,1]$, $x_0\in\mathbb{R}$, $R>0$ and $I :=]x_0-R, x_0+R[$. Given a function $g\in C_c(I)\cap C^2(I\setminus\{x_0\})$, we assume finiteness of the norms

$$|\!|\!| g |\!|\!|_l := \max_{0\leqslant k\leqslant l}\ \sup_{x\in I\setminus\{x_0\}} \left[|g^{(k)}(x)||x-x_0|^{-\gamma+k}\right] < \infty, \tag{4.194}$$

for $l\in\{0,1,2\}$. In particular, this implies that g is Hölder continuous at x_0 with $g(x_0)=0$.

Before we turn to the main theorem of this section, we first collect two additional ingredients. The first one is a version of Lemma 4.17 for functions satisfying Assumption 4.24. We quote a special case of [Sob17, Thm. 2.10] adapted to our situation.

Theorem 4.25. *Let g satisfy Assumption 4.24. Let $q \in]0,\gamma[$. Further, let X be a self-adjoint operator with dense domain $\mathcal{D}$ in a separable Hilbert space $\mathcal{H}$ and P be an orthogonal projection on $\mathcal{H}$ such that $P\mathcal{D} \subseteq \mathcal{D}$ and $PX(1_{\mathcal{H}} - P) \in \mathcal{T}_q$. Then*

$$\|g(PXP)P - Pg(X)\|_1 \leqslant C{|\!|\!|} g {|\!|\!|}_2 R^{\gamma-q} \|PX(1_{\mathcal{H}} - P)\|_q^q, \tag{4.195}$$

with a positive constant C independent of X, P, g and R.

We now combine this estimate with Lemma 4.17, in order to obtain a similar estimate for functions satisfying Assumption 4.23.

Lemma 4.26. *Let h satisfy Assumption 4.23 and be compactly supported. Then there exists $R_0 > 0$ such that for all $R \in]0, R_0]$ the function h can be decomposed as $h = \sum_{j=1}^N h_{R,j} + g_R$, with $h_{R,j}$ satisfying Assumption 4.24 with $x_0 = x_j$ and the same Hölder exponent $\gamma \in]0,1]$ as h for every $j \in \{1, \dots, N\}$ and $g_R \in C_c^2(\mathbb{R})$. Further, let $q \in]0,\gamma[$, X be a self-adjoint operator with dense domain $\mathcal{D}$ in a separable Hilbert space $\mathcal{H}$ and P be an orthogonal projection on $\mathcal{H}$ such that $P\mathcal{D} \subseteq \mathcal{D}$ and $PX(1_{\mathcal{H}} - P) \in \mathcal{T}_q$. Then there exist constants $C_j > 0$, $j \in \{0, \dots, N\}$, which are independent of X, P, h and R, such that*

$$\|h(PXP)P - Ph(X)\|_1 \leqslant \Big(\sum_{j=1}^N C_j {|\!|\!|} h_{R,j} {|\!|\!|}_2 R^{\gamma-q} + C_0 \max_{0\leqslant k\leqslant 2} \|g_R^{(k)}\|_\infty \Big) \|PX(1_{\mathcal{H}} - P)\|_q^q. \tag{4.196}$$

Proof. Let $g \in C_c^2(\mathbb{R})$ be a function such that $g(x_j) = h(x_j)$ for all $x_j \in \mathcal{X}$, $j \in \{1, \dots, N\}$. Then the function $h - g$ also satisfies Assumption 4.23 and $(h-g)(x_j) = 0$ for all $x_j \in \mathcal{X}$, $j \in \{1, \dots, N\}$. Let $R_0 > 0$ be small enough such that $]x_j - R_0, x_j + R_0[\subset U_j$ for every $j \in \{1, \dots, N\}$. For any $R \in]0, R_0]$ we write $h - g = \sum_{j=1}^N h_{R,j} + f_R$ with $h_{R,j}(x) := [h(x) - g(x)]\zeta((x - x_j)R^{-1})$, where $\zeta \in C_c^\infty(\mathbb{R})$ with $\zeta(x) = 1$ for all $x \in]-\frac{1}{2}, \frac{1}{2}[$ and $\zeta(x) = 0$ for all $x \notin]-1,1[$ as well as $\|\zeta\|_\infty = 1$. Then $f_R \in C_c^2(\mathbb{R})$ and $]x_j - R, x_j + R[\subset U_j$ for every $j \in \{1, \dots, N\}$. We now verify that each $h_{R,j}$ satisfies Assumption 4.24 with $x_0 = x_j$ and ${|\!|\!|} h_{R,j} {|\!|\!|}_2$ bounded uniformly in $R \in]0, R_0]$. Indeed, let $j \in \{1, \dots, N\}$ and $R \in]0, R_0]$ be arbitrary. Then for every $x \in]x_j - R, x_j + R[\setminus \{x_j\}$ the bound (4.193) applied to $h - g$ yields

$$\begin{aligned} &|h_{R,j}(x)||x - x_j|^{-\gamma} \\ &\quad = \big|\big[h(x) - g(x)\big]\zeta\big((x - x_j)R^{-1}\big)\big||x - x_j|^{-\gamma} \leqslant \big|h(x) - g(x)\big||x - x_j|^{-\gamma} \leqslant C \end{aligned} \tag{4.197}$$

and

$$\begin{aligned} &|h'_{R,j}(x)||x - x_j|^{-\gamma+1} \\ &\quad = \Big|\big[h'(x) - g'(x)\big]\zeta\big((x - x_j)R^{-1}\big) + \big[h(x) - g(x)\big]R^{-1}\zeta'\big((x - x_j)R^{-1}\big)\Big| |x - x_j|^{-\gamma+1} \\ &\quad \leqslant \big|h'(x) - g'(x)\big||x - x_j|^{-\gamma+1} + \|\zeta'\|_\infty \big|h(x) - g(x)\big| \frac{|x - x_j|}{R} |x - x_j|^{-\gamma} \leqslant C. \end{aligned} \tag{4.198}$$

The second derivative works in the same way. We now have the decomposition $h = \sum_{j=1}^N h_{R,j} + f_R + g = \sum_{j=1}^N h_{R,j} + g_R$, with $g + f_R =: g_R \in C_c^2(\mathbb{R})$.

It remains to apply Lemma 4.17 to g_R and Theorem 4.25 to each $h_{R,j}$ to obtain the desired estimate:

$$\begin{aligned}\|h(PXP)P - Ph(X)\|_1 &\leqslant \sum_{j=1}^{N} \|h_{R,j}(PXP)P - Ph_{R,j}(X)\|_1 + \|g_R(PXP)P - Pg_R(X)\|_1 \\ &\leqslant \Big(\sum_{j=1}^{N} C_j |\!|\!| h_{R,j} |\!|\!|_2 R^{\gamma-q} + C_0 \max_{0\leqslant k\leqslant 2} \|g_R^{(k)}\|_\infty\Big) \|PX(1_{\mathcal{H}} - P)\|_q^q. \end{aligned} \tag{4.199}$$

□

The second ingredient is an estimate for the coefficient $\mathfrak{W}_1$. For this, we need an estimate similar to (4.178). While this is easy to come by in the scalar-valued case, it is more difficult in the case with two matrix-valued symbols. In order to do so, we quote a simpler version of [Sob17, Thm. 2.4], which we will only need for a finite-dimensional Hilbert space.

Theorem 4.27. *Let g satisfy Assumption 4.24. Let $q \in]0, \gamma[$. Further, let X_1, X_2 be self-adjoint operators with dense domains $\mathcal{D}_1, \mathcal{D}_2$ in a separable Hilbert space $\mathcal{H}$ such that $\mathcal{D}_1 \cap \mathcal{D}_2$ is dense in $\mathcal{H}$ and $X_1 - X_2 \in \mathcal{T}_q$. Then*

$$\|g(X_1) - g(X_2)\|_1 \leqslant C |\!|\!| g |\!|\!|_2 R^{\gamma-q} \|X_1 - X_2\|_q^q, \tag{4.200}$$

with a positive constant C independent of X_1, X_2, g and R.

Now we turn to the coefficient. The next Lemma allows the matrix-valued symbols to depend on the space variable, even though this will not be needed in the main theorem.

Lemma 4.28. *Let g satisfy Assumption 4.24. Let $A_1, A_2 \in C_b^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{C}^{n\times n})$ be Hermitian matrix-valued symbols and let $\partial\Lambda$ and $\partial\Gamma$ have finite $(d-1)$-dimensional surface measure induced by Lebesgue measure on $\mathbb{R}^d$. Let $q \in]0, \gamma[$. Then there exists a constant $C > 0$, independent of g and R such that*

$$\big|\mathfrak{W}_1\big(\mathfrak{U}(g; A_1, A_2); \partial\Lambda, \partial\Gamma\big)\big| \leqslant C R^{\gamma-q} |\!|\!| g |\!|\!|_2. \tag{4.201}$$

Proof. As the surface measure of $\partial\Lambda$ and $\partial\Gamma$ is finite, it suffices to show

$$\sup_{(x,\xi)\in\partial\Lambda\times\partial\Gamma} \big|\big(\mathfrak{U}(g; A_1, A_2)\big)(x,\xi)\big| \leqslant C R^{\gamma-q} |\!|\!| g |\!|\!|_2. \tag{4.202}$$

As in the proof of Lemma 4.21, the strategy is to estimate pointwise, use the fact that $\frac{1}{t(1-t)} = \frac{1}{t} + \frac{1}{(1-t)}$ and consider the two integrals in (4.176) separately. For Hermitian matrices $M_1, M_2 \in \mathbb{C}^{n\times n}$, an application of Theorem 4.27 with $\mathcal{H} = \mathbb{C}^n$ and $X_1 = M_1$, $X_2 = M_2$ yields

$$\|g(M_1) - g(M_2)\|_1 \leqslant C |\!|\!| g |\!|\!|_2 R^{\gamma-q} \|M_1 - M_2\|_q^q, \tag{4.203}$$

with C independent of M_1, M_2, g and R. Here, the trace and q-norms are the appropriate matrix norms.

The first integral is as in (4.177), and we obtain

$$\begin{aligned}\int_0^1 &\frac{\operatorname{tr}_{\mathbb{C}^n}\left[g\big(A_1t+A_2(1-t)\big)-g(A_2)\right]}{t}\,\mathrm{d}t-\operatorname{tr}_{\mathbb{C}^n}[g(A_1)-g(A_2)]\\ &\leqslant C|\!|\!|g|\!|\!|_2R^{\gamma-q}\left(\int_0^1\frac{\|A_1t+A_2(1-t)-A_2\|_q^q}{t}\,\mathrm{d}t+\|A_1-A_2\|_q^q\right)\\ &\leqslant C|\!|\!|g|\!|\!|_2R^{\gamma-q}\big(\|A_1\|_q^q+\|A_2\|_q^q\big)\left(\int_0^1\frac{t^q}{t}\,\mathrm{d}t+1\right)\end{aligned}\tag{4.204}$$

by applying (4.203). We estimate the second integral in an analogous way and use the fact that the estimates hold for all $(x,\xi)\in\partial\Lambda\times\partial\Gamma$ to obtain the result. □

We are now ready to close the asymptotics.

Theorem 4.29. *Let $A_1,A_2\in C_b^\infty(\mathbb{R}^d,\mathbb{C}^{n\times n})$ be matrix-valued symbols, which only depend on the momentum variable ξ. We assume that A_2 is compactly supported in ξ. Let Λ be a bounded piece-wise C^1-admissible domain and Γ be a bounded piece-wise C^3-admissible domain. Let the function h satisfy Assumptions 4.23 and assume that $h(0)=0$. Then*

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}&\left[h\big(G_L(A_1,A_2;\Lambda,\Gamma)\big)\right]\\ &=L^d\Big[\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(\operatorname{Re}A_1)];\Lambda,\Gamma\big)+\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(\operatorname{Re}A_2)];\Lambda,\Gamma^c\big)\Big]\\ &\quad+L^{d-1}\log L\ \mathfrak{W}_1\big(\mathfrak{U}(h;\operatorname{Re}A_1,\operatorname{Re}A_2);\partial\Lambda,\partial\Gamma\big)\\ &\quad+o(L^{d-1}\log L),\end{aligned}\tag{4.205}$$

as $L\to\infty$. Here, the coefficients $\mathfrak{W}_0$ and $\mathfrak{W}_1$ were defined in (2.15) and (2.16), respectively, and the symbol $\mathfrak{U}$ in (2.32).

Proof. As the operator $G_L(A_1,A_2;\Lambda,\Gamma)$ is bounded, we can assume that h is compactly supported. By Lemma 4.26 there is some $R_0>0$ such that for every $R\in]0,R_0]$ we have the decomposition $h=\sum_{j=1}^N h_{R,j}+g_R$, with $h_{R,j}$ satisfying Assumption 4.24 with $x_0=x_j$ for every $j\in\{1,\dots,N\}$ and $g_R\in C_c^2(\mathbb{R})$. Let $\varepsilon>0$ and $R\in]0,R_0]$ be arbitrary. Then, as in the beginning of the proof of Theorem 4.22, we find a polynomial $p_{R,\varepsilon}$ such that

$$\max_{0\leqslant k\leqslant 2}\|g_{R,\varepsilon}^{(k)}\|_\infty<\varepsilon\tag{4.206}$$

for $g_{R,\varepsilon}:=g_R-p_{R,\varepsilon}$. The supremum norm in (4.206) is the one on $\operatorname{supp}h$, the support of the function h (which contains $\operatorname{supp}g_R$).

We now study the function $h_{R,\varepsilon}:=h-p_{R,\varepsilon}=\sum_{j=1}^N h_{R,j}+g_{R,\varepsilon}$. As it is decomposed in the same manner as h in Lemma 4.26, the estimate from Lemma 4.26 holds with $h=h_{R,\varepsilon}$, $g_R=g_{R,\varepsilon}$, $X=G_L\big(A_1,A_2;\mathbb{R}^d,\Gamma\big)$, $P=\mathbf{1}_\Lambda$ and arbitrary $q\in]0,\gamma[$. We obtain

$$\begin{aligned}\Big\|h_{R,\varepsilon}&\big(G_L(A_1,A_2)\big)-\mathbf{1}_\Lambda h_{R,\varepsilon}\big(G_L(A_1,A_2;\mathbb{R}^d,\Gamma)\big)\mathbf{1}_\Lambda\Big\|_1\\ &\leqslant\Big(\sum_{j=1}^N C_j|\!|\!|h_{R,j}|\!|\!|_2R^{\gamma-q}+C_0\max_{0\leqslant k\leqslant 2}\|g_{R,\varepsilon}^{(k)}\|_\infty\Big)\Big\|\mathbf{1}_\Lambda G_L(A_1,A_2;\mathbb{R}^d,\Gamma)\mathbf{1}_{\Lambda^c}\Big\|_q^q.\end{aligned}\tag{4.207}$$

As the symbols A_1 and A_2 only depend on the variable ξ, the functional calculus yields the following equality

$$D_L\big(h_{R,\varepsilon}(\operatorname{Re}A_1),h_{R,\varepsilon}(\operatorname{Re}A_2)\big)=\mathbf{1}_\Lambda h_{R,\varepsilon}\big(G_L(A_1,A_2;\mathbb{R}^d,\Gamma)\big)\mathbf{1}_\Lambda.\tag{4.208}$$

With this and Lemma 3.8 we conclude from (4.207) that

$$\Big\| h_{R,\varepsilon}\big(G_L(A_1,A_2)\big) - D_L\big(h_{R,\varepsilon}(\operatorname{Re} A_1), h_{R,\varepsilon}(\operatorname{Re} A_2)\big)\Big\|_1 \leqslant C(R^{\gamma-q}+\varepsilon)L^{d-1}\log L, \tag{4.209}$$

where the constant C is independent of L, R and ε. Here we additionally used (4.206) and that $|\!|\!| h_{R,j} |\!|\!|_2$ is bounded uniformly in $R \in]0, R_0]$ (cf. the proof of Lemma 4.26). Using that

$$\begin{aligned}
&\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h(G_L(A_1,A_2)) - D_L\big(h(\operatorname{Re} A_1), h(\operatorname{Re} A_2)\big)\big] \\
&\qquad \leqslant \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[p_{R,\varepsilon}\big(G_L(A_1,A_2)\big) - D_L\big(p_{R,\varepsilon}(\operatorname{Re} A_1), p_{R,\varepsilon}(\operatorname{Re} A_2)\big)\big] \\
&\qquad\quad + \big\| h_{R,\varepsilon}\big(G_L(A_1,A_2)\big) - D_L\big(h_{R,\varepsilon}(\operatorname{Re} A_1), h_{R,\varepsilon}(\operatorname{Re} A_2)\big)\big\|_1,
\end{aligned}\tag{4.210}$$

and that the asymptotic formula is already established for polynomials, we see that

$$\begin{aligned}
&\limsup_{L\to\infty} \frac{\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(G_L(A_1,A_2)\big) - D_L\big(h(\operatorname{Re} A_1), h(\operatorname{Re} A_2)\big)\big]}{L^{d-1}\log L} \\
&\qquad\qquad \leqslant \mathfrak{W}_1(p_{R,\varepsilon}) + C(R^{\gamma-q}+\varepsilon),
\end{aligned}\tag{4.211}$$

where $\mathfrak{W}_1(p_{R,\varepsilon}) := \mathfrak{W}_1\big(\mathfrak{U}(p_{R,\varepsilon}; \operatorname{Re} A_1, \operatorname{Re} A_2); \partial\Lambda, \partial\Gamma\big)$. For the coefficient $\mathfrak{W}_1(h_{R,\varepsilon})$, Lemmas 4.21 and 4.28 yield

$$|\mathfrak{W}_1(h_{R,\varepsilon})| \leqslant \sum_{j=1}^{N} |\mathfrak{W}_1(h_{R,j})| + |\mathfrak{W}_1(g_{R,\varepsilon})| \leqslant C(R^{\gamma-q}+\varepsilon), \tag{4.212}$$

where the constant C is again independent of L, R and ε, and we again used (4.206) and that $|\!|\!| h_{R,j} |\!|\!|_2$ is bounded uniformly in $R \in]0, R_0]$. Therefore,

$$\mathfrak{W}_1(p_{R,\varepsilon}) \leqslant \mathfrak{W}_1(h) + |\mathfrak{W}_1(h_{R,\varepsilon})| \leqslant \mathfrak{W}_1(h) + C(R^{\gamma-q}+\varepsilon). \tag{4.213}$$

Combining this with (4.207), we obtain

$$\limsup_{L\to\infty} \frac{\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(G_L(A_1,A_2)\big) - D_L\big(h(\operatorname{Re} A_1), h(\operatorname{Re} A_2)\big)\big]}{L^{d-1}\log L} \leqslant \mathfrak{W}_1(h) + C(R^{\gamma-q}+\varepsilon). \tag{4.214}$$

The corresponding lower bound for the liminf is found in the same way. As R and ε are arbitrarily small, we conclude

$$\lim_{L\to\infty} \frac{\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(G_L(A_1,A_2)\big) - D_L\big(h(\operatorname{Re} A_1), h(\operatorname{Re} A_2)\big)\big]}{L^{d-1}\log L} = \mathfrak{W}_1(h). \tag{4.215}$$

As the symbols A_1 and A_2 only depend on the variable ξ, the operator $D_L\big(h(\operatorname{Re} A_1), h(\operatorname{Re} A_2)\big)$ gives rise to the volume terms by integrating its kernel along the diagonal, and we obtain the desired asymptotic formula

$$\begin{aligned}
&\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(G_L(A_1,A_2;\Lambda,\Gamma)\big)\big] \\
&\qquad = L^d\big[\mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(\operatorname{Re} A_1)]; \Lambda, \Gamma\big) + \mathfrak{W}_0\big(\operatorname{tr}_{\mathbb{C}^n}[h(\operatorname{Re} A_2)]; \Lambda, \Gamma^c\big)\big] \\
&\qquad\quad + L^{d-1}\log L\ \mathfrak{W}_1\big(\mathfrak{U}(h; \operatorname{Re} A_1, \operatorname{Re} A_2); \partial\Lambda, \partial\Gamma\big) \\
&\qquad\quad + o(L^{d-1}\log L),
\end{aligned}\tag{4.216}$$

as $L \to \infty$. □

Remark 4.30. The condition that Γ is bounded in Theorems 4.14, 4.22 and 4.29 can be replaced by the condition that A_1 is compactly supported in the second variable.

To see this, note that the asymptotics for polynomials is already established under this condition (cf. Theorem 4.5 and Corollary 4.6) and treat A_1 analogously to A_2 throughout the relevant proofs in the Sections 4.4 - 4.6. We note here that this is possible, because we never used the fact that the complement of Γ^c is bounded.

The condition that Γ is bounded in the estimates for the coefficient (Lemmas 4.13, 4.21 and 4.28) is no longer necessary, as with A_1 and A_2 being compactly supported in the second variable the symbol $\mathfrak{U}(g; A_1, A_2)$ is also compactly supported in the second variable.

Remark 4.31. Closing the asymptotics for test functions as in Theorem 4.29 is easier in the case that $A_2 = 0$ and the test function h is constant on the range of the symbol A_1, i.e. if $(h(A_1))(\xi) = z$ for every $\xi \in \mathbb{R}^d$ and some $z \in \mathbb{C}$. In this case, the volume term vanishes for the modified function $\tilde{h} = h - z$ and the operator difference on the right-hand side of (4.207) only consists of a single operator. Therefore, it is easier to obtain the corresponding estimate. The above property is in particular fulfilled in the scalar-valued case corresponding to the Laplacian [LSS14], where $A_1 = 1$, $A_2 = 0$ and h is one of the entropy functions satisfying $h(0) = 0 = h(1)$. The corresponding closing of the asymptotics [LSS14, starting after (11)] does not make use of any of the results from [Sob17] which we use in the present chapter. However, the more involved approach chosen in Theorem 4.29 will be required for the application to the free Dirac operator in the following chapter. This is due to the presence of the smooth cut-off function φ_{E_F} in the symbol, see (2.43) for its definition.

Remark 4.32. Sometimes it is useful to consider domains Λ which are not bounded themselves but only have bounded complement, especially for applications considering the relative entanglement, see e.g. [LSS16, LSS17, Sob19, FLS24]. Then an asymptotic formula as in Theorem 4.29 does not hold, as the operator $h(G_L(A_1, A_2; \Lambda, \Gamma))$ is in general not trace class. Nevertheless, one obtains the following interim result, cf. (4.215),

$$\lim_{L\to\infty} \frac{\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[h\big(G_L(A_1, A_2; \Lambda, \Gamma)\big) - D_L\big(h(\operatorname{Re} A_1), h(\operatorname{Re} A_2); \Lambda, \Gamma\big)\right]}{L^{d-1}\log L}$$
$$= \mathfrak{W}_1\big(\mathfrak{U}(h; \operatorname{Re} A_1, \operatorname{Re} A_2); \partial\Lambda, \partial\Gamma\big), \quad (4.217)$$

under the same assumptions as in Theorem 4.29, except that now Λ^c needs to be bounded instead of Λ.

Proof of Remark 4.32. The crucial part is to establish (4.217) for polynomial test functions. Recalling that the symbols A_1 and A_2 in Theorem 4.29 only depend on the variable ξ, we see that this is precisely the statement of Corollary 4.7. The extension to the more general class of test functions mirrors the proof of Theorem 4.29 up to equation (4.215). □

CHAPTER 5

The Widom–Sobolev formula for the free Dirac Operator

Context: This chapter coincides mostly, in both content and writing, with the article [BM25] which was written in collaboration with Peter Müller. The organisation of the content has been slightly altered to better fit into the present thesis and the discussion of results in Section 5.1 has been extended.

Content: In this chapter we apply the results from Chapter 4 to the free Dirac operator. We first present the main result and discuss the strategy of the proof. We then split the proof into several cases depending on the constellation of the chosen Fermi energy E_F and mass m. In some of these cases an enhanced area law holds. In these cases we reduce the proof to an application of Theorem 4.29. In the other cases we use the estimates obtained in Chapter 3 to show that at most an area law holds.

5.1. Discussion of results and strategy of the proof

One of the primary applications of the Widom–Sobolev formula for scalar-valued symbols [Sob13, Sob17] is to obtain a logarithmically enhanced scaling law for the entanglement entropy of the free Fermi gas, see [LSS14]. In this case the single-particle Hamiltonian is given by the negative Laplacian. It is natural to ask how the situation changes when the Laplacian is replaced by its relativistic counterpart, the free Dirac operator. The goal of this chapter is to answer this question by obtaining an enhanced area law in the case of the free Dirac operator from the results established in Chapter 4. As described in Section 2.2 we consider a smoothly cut-off version of the Fermi projection at a given Fermi energy E_F. We recall its definition in (2.43). The compact support of the function $\chi_{E_F}^{(b)}$ guarantees that the operator

$$h\big(\mathbf{1}_{\Omega_L}\chi_{E_F}^{(b)}(D)\mathbf{1}_{\Omega_L}\big) \tag{5.1}$$

is trace class for a given bounded domain $\Omega \subset \mathbb{R}^d$. As the function $\chi_{E_F}^{(b)}$ has range $\operatorname{ran}\chi_{E_F}^{(b)} = [0,1]$, a comparison with the asymptotic expansion in Theorem 4.29 shows, that we can not expect the leading volume term, of the asymptotic trace expansion of (5.1), to vanish in general. Even for the special case of the entropy functions, where $h(0) = 0 = h(1)$. Therefore, we require the more complex version of closing the asymptotics as employed in Theorem 4.29 opposed to the easier one employed in the case of the Laplacian [LSS14], see Remark 4.31 for more details. To still obtain a vanishing coefficient for the volume term in the main theorem of the present chapter, we make use of the following reduction scheme. Given a suitable bounded domain $\Lambda \subset \mathbb{R}^d$ we consider a larger bounded domain $\Lambda' \subset \mathbb{R}^d$ such that Λ is well inside Λ', i.e. we have $\operatorname{dist}(\Lambda, \partial\Lambda') > 0$. This guarantees that the boundaries of the domains are disjoint and we have $\partial\Lambda \subset \Lambda'$. The difference of volumes, i.e. Lebesgue measures on $\mathbb{R}^d$,

$$|\Lambda| + |\Lambda' \setminus \Lambda| - |\Lambda'| \tag{5.2}$$

vanishes, and for the difference of the boundaries we obtain

$$\mathbf{1}_{\partial\Lambda} + \mathbf{1}_{\partial(\Lambda'\setminus\Lambda)} - \mathbf{1}_{\partial\Lambda'} = \mathbf{1}_{\partial\Lambda} + \mathbf{1}_{\partial\Lambda'} + \mathbf{1}_{\partial\Lambda} - \mathbf{1}_{\partial\Lambda'} = 2\mathbf{1}_{\partial\Lambda}. \tag{5.3}$$

Considering this difference therefore allows us to isolate the contribution of the boundary $\partial\Lambda$. The corresponding enhanced area law is the content of the following theorem, the main result of the present chapter.

Theorem 5.1. *Let $\Lambda \subset \Lambda'$ be bounded piece-wise C^1-admissible domains in $\mathbb{R}^d$ in the sense of Definition* 2.2 *and such that* $\operatorname{dist}(\Lambda, \partial\Lambda') > 0$. *Consider the Dirac operator* (2.34) *with mass $m \geqslant 0$ and fix a Fermi energy $E_F \in \mathbb{R}$ and an ultraviolet cut-off parameter $b \geqslant 0$. Let $h \in C(\mathbb{R})$ satisfy Assumption* 4.23 *and $h(0) = 0$. Then the asymptotic trace formula*

$$\frac{1}{n}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[h\big(\mathbf{1}_{\Lambda_L}\chi_{E_F}^{(b)}(D)\mathbf{1}_{\Lambda_L}\big) + h\big(\mathbf{1}_{\Lambda'_L\setminus\Lambda_L}\chi_{E_F}^{(b)}(D)\mathbf{1}_{\Lambda'_L\setminus\Lambda_L}\big) - h\big(\mathbf{1}_{\Lambda'_L}\chi_{E_F}^{(b)}(D)\mathbf{1}_{\Lambda'_L}\big)\Big]$$
$$= L^{d-1}\log L\; W(h,\Lambda,E_F,m) + o(L^{d-1}\log L) \quad (5.4)$$

holds as $L \to \infty$. The coefficient $W(h,\Lambda,E_F,m)$ is independent of the cut-off parameter b, the domain Λ' and the spinor dimension $n = n_d$. Moreover:

(a) *If $|E_F| > m$, then the coefficient of this enhanced area law is given by*

$$W(h,\Lambda,E_F,m) := \frac{\Phi(\Lambda,E_F,m)}{(2\pi)^2}\int_0^1 \frac{h(t)-h(1)t}{t(1-t)}\,\mathrm{d}t \quad (5.5)$$

with the geometric factor

$$\Phi(\Lambda,E_F,m) := \begin{cases} 2|\partial\Lambda|, & \text{if } d = 1,\\ \dfrac{1}{(2\pi)^{d-1}}\displaystyle\int_{\partial\Lambda}\int_{\partial B_{p_F}} |\nu_{\partial\Lambda}(x)\cdot\nu_{\partial B_{p_F}}(\xi)|\,\mathrm{d}S(\xi)\mathrm{d}S(x), & \text{if } d \geqslant 2, \end{cases} \quad (5.6)$$

where, in one dimension, $|\partial\Lambda|$ is the number of boundary points of Λ. In dimensions $d \geqslant 2$, we write $B_{p_F} := B_{p_F}(0)$, where $p_F := \sqrt{E_F^2 - m^2}$ is the relativistic Fermi momentum, and $\nu_{\partial\Lambda}$, resp. $\nu_{\partial B_{p_F}}$, denotes the vector field of exterior unit normals in $\mathbb{R}^d$ to $\partial\Lambda$, resp. ∂B_{p_F}. We write $\mathrm{d}S$ for integration with respect to the $(d-1)$-dimensional surface measure induced by Lebesgue measure in $\mathbb{R}^d$.

(b) *If $|E_F| \leqslant m \neq 0$, then $W(h,\Lambda,E_F,m) = 0$, and the next term in the asymptotic expansion is of order $O(L^{d-1})$ as $L \to \infty$.*

(c) *If $E_F = m = 0$, then the behaviour depends on the dimension. If $d = 1$ an enhanced area law holds with the same coefficient* (5.5) *and* (5.6) *as in* (a). *If instead $d \geqslant 2$, the situation is as in* (b).

Remark 5.2. (a) We note that in $d = 1$ the geometric factor $\Phi(\Lambda,E_F,m) = 2|\Lambda|$ and subsequently the coefficient $W(h,\Lambda,E_F,m)$ are actually independent of the Fermi energy E_F and the mass m. In $d \geqslant 2$ the geometric factor can also be computed explicitly [LSS14] as

$$\Phi(\Lambda,E_F,m) = \frac{2}{\Gamma\big(\frac{d+1}{2}\big)}\Big(\frac{p_F^2}{4\pi}\Big)^{\frac{d-1}{2}}|\partial\Lambda|, \quad (5.7)$$

where Γ denotes Euler's gamma function.

(b) For the Rényi entropy functions h_α, $\alpha \in \,]0,\infty[\,$, the coefficient $W(h,\Lambda,E_F,m)$ can also be computed explicitly as $W(h_\alpha,\Lambda,E_F,m) = \frac{1+\alpha}{24\alpha}\Phi(\Lambda,E_F,m)$, see [LSS14].

(c) For positive mass $m > 0$, $|E_F| > m$ and comparatively small Fermi momentum, i.e. $|E_F| - m \ll m$, the geometric factor $\Phi(\Lambda,E_F,m)$ resembles the one in the corresponding asymptotic expansion for the Laplacian with non-relativistic Fermi momentum defined in terms of the kinetic energy and given by $p_c^2 := 2m(|E_F| - m)$. More precisely, we have $\Phi(\Lambda, E_F, m) = J(\partial B_{p_c}, \partial\Lambda)\big[1 + O\big((|E_F| - m)/m\big)\big]$, where the function $J(\cdot,\cdot)$ is the corresponding geometric factor defined in [LSS14, Eq. (2)].

(d) The statements of Theorem 5.1 remain true in the case where the bigger volume Λ' is unbounded but has a bounded complement, see Remark 4.32. In particular, one may set $\Lambda' = \mathbb{R}^d$. This allows to relate the operators within the trace of (5.4) to the operators studied in, e.g., [LSS16, LSS17, Sob19, FLS24], where the volume term is subtracted directly.

(e) The factor $\frac{1}{n}$ on the left-hand side of (5.4) should be read as $\frac{1}{2}\frac{1}{n/2}$ with the first factor $\frac{1}{2}$ accounting for the fact that the boundary of Λ is counted twice by the trace. The second factor $\frac{1}{n/2}$ accounts for the number of spinor dimensions which contribute to the discontinuity in momentum space. As it turns out, each of these dimensions contributes the same amount to the enhanced area law.

We can directly compare the obtained result with the earlier result for the Laplacian [LSS14]. In the case of positive mass $m > 0$, it is not surprising that we do not obtain an enhanced area law, if the Fermi energy lies in the spectral gap, i.e. $E_F \in [-m, m]$. This agrees with the situation for the Laplacian, where a cut-off outside the absolutely continuous spectrum, i.e. $E_F \leqslant 0$, also does not yield a logarithmic enhancement. In both cases, this can be attributed to the fact that this cut-off does not lead to a discontinuity of the corresponding symbol. If we instead have $|E_F| > m$, the Fermi projection yields a discontinuity of the symbol at the boundary of the ball B_{p_F}, the relativistic Fermi ball. This is again similar to the case of the Laplacian, where a cut-off at positive Fermi energy $E_F > 0$ leads to a discontinuity of the symbol at the boundary of the non-relativistic Fermi ball B_{p_c}. But whereas for the Laplacian the relevant region in momentum space is always contained in the Fermi ball B_{p_c}, this is not the case for the free Dirac operator. For positive Fermi energies $E_F > m$, the symbol takes on non-zero values on both sides of the discontinuity. Still, the obtained coefficients for the enhanced area laws agree; up to the difference between the Fermi momentums p_F and p_c. This also explains Remark 5.2(c), as the comparison of the coefficients reduces to the well-known comparison of the relativistic and non-relativistic Fermi momentums. In the case $E_F = m = 0$, we are faced with a situation without a counterpart in the Laplacian case. Here, the symbol turns out to be discontinuous at the origin, a 0-dimensional set instead of the $(d-1)$-dimensional boundary of a ball. This leads to the different cases depending on the spatial dimension d in Theorem 5.1. As this type of discontinuity seems specific to the structure of the Dirac operator, not many mathematical results are available on such symbols. Therefore, studying this situation is of particular interest, which we do to some degree in the present chapter and far more extensively in Chapter 6.

We now give a short overview of the strategy of the proof of Theorem 5.1: We first evaluate

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[h\big(\mathbf{1}_{\Omega_L}\chi_{E_F}^{(b)}(D)\mathbf{1}_{\Omega_L}\big)\Big] \tag{5.8}$$

for a single bounded piece-wise C^1-admissible domain Ω, representing either Λ, Λ' or $\Lambda'\setminus\Lambda$. As discussed in Remark 2.10 (b), we rewrite this in terms of the operator with symbol $\chi_{E_F}^{(b)}(D)$, i.e.

$$\chi_{E_F}^{(b)}(D) = \operatorname{Op}_1\big(\chi_{E_F}^{(b)}(D)\big). \tag{5.9}$$

As the symbol $\chi_{E_F}^{(b)}(D)$ only depends on momentum space, we have, recalling the definition of the operator Op_L in (2.22),

$$U_L\mathbf{1}_{\Omega_L}\operatorname{Op}_1\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_{\Omega_L}U_L^{-1} = \mathbf{1}_\Omega\operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_\Omega, \tag{5.10}$$

where the dilatation U_L on $L^2(\mathbb{R}^d)\otimes\mathbb{C}^n$ is given by $(U_Lu)(x) := L^{\frac{d}{2}}u(Lx)$ for all $u \in L^2(\mathbb{R}^d)\otimes\mathbb{C}^n$, i.e. the operators $\mathbf{1}_{\Omega_L}\operatorname{Op}_1\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_{\Omega_L}$ and $\mathbf{1}_\Omega\operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_\Omega$ are unitarily equivalent. Therefore, we infer

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[h\big(\mathbf{1}_{\Omega_L}\operatorname{Op}_1\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_{\Omega_L}\big)\Big] = \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[h\big(\mathbf{1}_{\Omega}\operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_{\Omega}\big)\Big] \tag{5.11}$$

and it remains to evaluate

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[h\big(\mathbf{1}_{\Omega}\operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_{\Omega}\big)\Big]. \tag{5.12}$$

In the cases where we establish an enhanced area law, we show that (5.12) yields a volume term which is proportional to $|\Omega|$, an enhanced area term with coefficient $W(h,\Omega,E_F,m)$ and an error term of order $o(L^{d-1}\log L)$. The crucial part will be to study the symbol $\chi_{E_F}^{(b)}(D)$ and write it in such a way that the Widom–Sobolev formula for matrix-valued symbols, Theorem 4.29 respectively Remark 4.30, can be applied. In general, an application of (2.42) with $a=\chi_{E_F}^{(b)}$ yields

$$\chi_{E_F}^{(b)}(D(\xi)) = \frac{1}{2}\Big(\big(\chi_{E_F}^{(b)}\big)_+ + \big(\chi_{E_F}^{(b)}\big)_-\Big)(\xi)\mathbb{1}_n + \frac{1}{2}\Big(\big(\chi_{E_F}^{(b)}\big)_+ - \big(\chi_{E_F}^{(b)}\big)_-\Big)(\xi)\frac{D(\xi)}{E(\xi)}, \tag{5.13}$$

where $\big(\chi_{E_F}^{(b)}\big)_\pm$ are defined as in (2.41). The properties of these functions depend on the parameters E_F and m and will be investigated in the respective sections. After applying the Widom–Sobolev formula, it remains to explicitly calculate the resulting coefficients. While doing so, we will frequently use the property that $h(0)=0$ for the function h in Theorem 5.1 without explicitly stating it.

In the cases without an enhanced area law, we estimate the trace norm

$$\Big\|h\Big(\mathbf{1}_{\Omega}\operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_{\Omega}\Big) - \mathbf{1}_{\Omega}\operatorname{Op}_L\Big(h\big(\chi_{E_F}^{(b)}(D)\big)\Big)\mathbf{1}_{\Omega}\Big\|_1 \tag{5.14}$$

and show that it only yields an area term. To do so, we first reduce the question to estimating a suitable Schatten–von Neumann norm by applying Lemma 4.26. In the case $|E_F|\leqslant m\neq 0$ the corresponding symbol turns out to be smooth, and the estimate for the Schatten–von Neumann norm follows from Lemma 3.6. In the case $E_F=m=0$ with $d\geqslant 2$, the symbol turns out to be discontinuous at the origin, and we require the appropriate estimate contained in Lemma 3.9.

We start with the case $|E_F|>m$ in Section 5.2, continue with the case $|E_F|\leqslant m\neq 0$ in Section 5.3 and conclude with the case $E_F=m=0$ in Section 5.4. Afterwards, we prove Theorem 5.1 in Section 5.5 by applying the results to $\Omega=\Lambda$, $\Omega=\Lambda'$ and $\Omega=\Lambda'\setminus\Lambda$ and by showing that the respective volume terms add up to zero.

5.2. The case $|E_F|>m$

In this case we show that the symbol $\chi_{E_F}^{(b)}(D)$ is discontinuous precisely at the boundary of the ball B_{p_F}. Hence, we define our cut-off region in momentum space $\Gamma := \{\xi\in\mathbb{R}^d:\ E(\xi)<|E_F|\} = B_{p_F}$ as this ball. This is clearly a bounded piece-wise C^3-domain and therefore satisfies the requirements of Theorem 4.29. We now show the desired asymptotic formula for an arbitrary bounded piece-wise C^1-admissible domain Ω. The next lemma treats the case $E_F<-m$. The case $E_F>m$ will be tackled in Lemma 5.4.

Lemma 5.3. *Let h be as in Theorem 5.1, Ω be a bounded piece-wise C^1-admissible domain, $b\geqslant 0$, $E_F\in\mathbb{R}$ and $m\geqslant 0$ such that $E_F<-m$. Then we have*

$$\begin{aligned}\frac{2}{n}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}&\Big[h\Big(\mathbf{1}_{\Omega}\operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_{\Omega}\Big)\Big]\\ &= L^d\,V_-(h,b,E_F,m)|\Omega| + L^{d-1}\log L\,W(h,\Omega,E_F,m) + o(L^{d-1}\log L),\end{aligned} \tag{5.15}$$

as $L \to \infty$, where

$$V_-(h,b,E_F,m) := \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\big[h\circ\big(\chi_{E_F}^{(b)}\big)_-\big](\xi)\,\mathrm{d}\xi \tag{5.16}$$

is independent of n and Ω.

Proof. If $E_F < -m$, we have $\big(\chi_{E_F}^{(b)}\big)_+(\xi) = 0$ and

$$\big(\chi_{E_F}^{(b)}\big)_-(\xi) = 1_{\Gamma^c}(\xi)\varphi\big(-E(\xi)+b\big) =: 1_{\Gamma^c}(\xi)\tilde{\varphi}^{(b)}(\xi) \tag{5.17}$$

for the functions in (5.13), which allows us to rewrite

$$h\Big(\mathbf{1}_\Omega\operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_\Omega\Big) = h\Big(\mathbf{1}_\Omega\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\operatorname{Op}_L\big(\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big)\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Omega\Big). \tag{5.18}$$

Recall that the matrix-valued symbol $\frac{D}{E}$ is smooth, except at the origin in the case $m = 0$. Due to the presence of the projection $\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})$, we can modify the function $\tilde{\varphi}^{(b)}$ inside of Γ without changing (5.18). In particular, we can replace $\tilde{\varphi}^{(b)}$ by a smooth and compactly supported function $\varphi^{(b)} \in C_c^\infty(\mathbb{R}^d)$ with $\varphi^{(b)}(0) = 0$, as $\overline{\Gamma^c}\cap\{0\} = \varnothing$. Then the symbol $\frac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \frac{D}{E})$ is smooth, bounded and compactly supported. As Ω is a bounded piece-wise C^1-admissible domain, Γ is a bounded piece-wise C^3-admissible domain and h satisfies Assumption 4.23 with $h(0) = 0$, all the requirements of Theorem 4.29 are fulfilled, and an application of this theorem with $A_1 := 0, A_2 := \frac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \frac{D}{E})$ yields the asymptotic expansion

$$\begin{aligned}
&\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[h\Big(\mathbf{1}_\Omega\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\operatorname{Op}_L\big(\tfrac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big)\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\mathbf{1}_\Omega\Big)\Big]\\
&\qquad = L^d\,\mathfrak{W}_0\Big(\operatorname{tr}_{\mathbb{C}^n}\big[h\big(\tfrac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big)\big];\Omega,\Gamma^c\Big)\\
&\qquad\quad + L^{d-1}\log L\,\mathfrak{W}_1\Big(\mathfrak{U}\big(h;0,\tfrac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big);\partial\Omega,\partial\Gamma\Big)\\
&\qquad\quad + o(L^{d-1}\log L),
\end{aligned} \tag{5.19}$$

as $L \to \infty$. For the readers convenience we recall the definitions of the occurring coefficients. For a bounded scalar-valued symbol a and admissible domains Ω, Ξ with 1_Ω and $1_\Xi a$ having compact support we have

$$\mathfrak{W}_0(a;\Omega,\Xi) = \frac{|\Omega|}{(2\pi)^d}\int_\Xi a(\xi)\,\mathrm{d}\xi \tag{5.20}$$

and

$$\mathfrak{W}_1(a;\partial\Omega,\partial\Xi) = \begin{cases} |\partial\Omega|\displaystyle\sum_{\xi\in\partial\Xi} a(\xi), & \text{for } d = 1,\\[2ex] \dfrac{1}{(2\pi)^{d-1}}\displaystyle\int_{\partial\Omega}\int_{\partial\Xi} a(\xi)\,|\nu_{\partial\Omega}(x)\cdot\nu_{\partial\Xi}(\xi)|\,\mathrm{d}S(\xi)\,\mathrm{d}S(x), & \text{for } d \geqslant 2.\end{cases} \tag{5.21}$$

We note that if the symbol a is equal to some constant a_0 on $\partial\Xi$ and $\partial\Xi = \partial B_{p_F}$, then

$$\mathfrak{W}_1(a;\partial\Omega,\partial\Gamma) = a_0\Phi(\Omega,E_F,m), \tag{5.22}$$

where $\Phi(\Omega,E_F,m)$ is defined in Theorem 5.1. The symbol $\mathfrak{U}(g;A_1,A_2)$ appearing in the first argument of the coefficient $\mathfrak{W}_1$ in (5.19) is given by

$$\mathfrak{U}(g;A_1,A_2) = \frac{1}{(2\pi)^2}\int_0^1\frac{\operatorname{tr}_{\mathbb{C}^n}\big[g\big(A_1t + A_2(1-t)\big) - g(A_1)t - g(A_2)(1-t)\big]}{t(1-t)}\,\mathrm{d}t \tag{5.23}$$

and depends on a Hölder continuous function $g : \mathbb{R}\to\mathbb{C}$ and bounded matrix-valued symbols A_1, A_2.

In order to compute the matrix traces in the coefficients, it will be convenient to diagonalise the symbol $\frac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \frac{D}{E}) = \frac{1}{2}U^{-1}\varphi^{(b)}(\mathbb{1}_n - \beta)U$ argument-wise as in (2.42). This gives for any $z \in \mathbb{C}$

$$\begin{aligned}\operatorname{tr}_{\mathbb{C}^n}\Big[h\big(\tfrac{z}{2}\varphi^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big)\Big] &= \operatorname{tr}_{\mathbb{C}^n}\Big[U^{-1}h\big(\tfrac{z}{2}\varphi^{(b)}(\mathbb{1}_n - \beta)\big)U\Big]\\ &= \operatorname{tr}_{\mathbb{C}^n}\begin{pmatrix}0 & 0\\ 0 & h(z\varphi^{(b)})\mathbb{1}_{\frac{n}{2}}\end{pmatrix} = \frac{n}{2}\,h(z\varphi^{(b)})\end{aligned} \tag{5.24}$$

and implies for $z = 1-t$ and $z = 1$, respectively,

$$\begin{aligned}&\mathfrak{U}\big(h; 0, \tfrac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big)\\ &\quad= \frac{1}{(2\pi)^2}\int_0^1 \frac{\operatorname{tr}_{\mathbb{C}^n}\big[h\big(\frac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \frac{D}{E})(1-t)\big) - h\big(\frac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \frac{D}{E})\big)(1-t)\big]}{t(1-t)}\,\mathrm{d}t\\ &\quad= \frac{n}{2}\frac{1}{(2\pi)^2}\int_0^1 \frac{h\big(\varphi^{(b)}(1-t)\big) - h(\varphi^{(b)})(1-t)}{t(1-t)}\,\mathrm{d}t = \frac{n}{2}\,\mathfrak{A}(h;\varphi^{(b)}),\end{aligned} \tag{5.25}$$

where we recall

$$\mathfrak{A}(h;a) = \frac{1}{(2\pi)^2}\int_0^1 \frac{h(at) - h(a)t}{t(1-t)}\,\mathrm{d}t \tag{5.26}$$

for a bounded scalar-valued symbol a.

We conclude from (5.24) with $z = 1$ that

$$\begin{aligned}&\mathfrak{W}_0\Big(\operatorname{tr}_{\mathbb{C}^n}\big[h\big(\tfrac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big)\big]; \Omega, \Gamma^c\Big)\\ &\quad= \frac{n}{2}\,\mathfrak{W}_0\big(h(\varphi^{(b)}); \Omega, \Gamma^c\big) = \frac{n}{2}\frac{|\Omega|}{(2\pi)^d}\int_{\Gamma^c}\big(h(\varphi^{(b)})\big)(\xi)\,\mathrm{d}\xi = \frac{n}{2}\,|\Omega| V_-(h, b, E_F, m),\end{aligned} \tag{5.27}$$

where the last equality rests on (5.17).

Now we return to (5.25). Since $\varphi^{(b)}|_{\partial\Gamma} = 1$, we see that $\mathfrak{A}(h;\varphi^{(b)})|_{\partial\Gamma} = \frac{1}{(2\pi)^2}\int_0^1 \frac{h(t)-h(1)t}{t(1-t)}\,\mathrm{d}t$ is also constant and, thus we infer from (5.22) that

$$\begin{aligned}\mathfrak{W}_1\Big(\mathfrak{U}\big(h; 0, \tfrac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big); \partial\Omega, \partial\Gamma\Big) &= \frac{n}{2}\,\mathfrak{W}_1\big(\mathfrak{A}(h;\varphi^{(b)}); \partial\Omega, \partial\Gamma\big)\\ &= \frac{n}{2}\frac{1}{(2\pi)^2}\int_0^1 \frac{h(t) - h(1)t}{t(1-t)}\,\mathrm{d}t\ \Phi(\Omega, E_F, m) = \frac{n}{2}\,W(h, \Omega, E_F, m).\end{aligned} \tag{5.28}$$

Therefore, the claim follows with (5.27) and (5.19). $\square$

Lemma 5.4. *Let h be as in Theorem 5.1, Ω be a bounded piece-wise C^1-admissible domain, $b \geqslant 0$, $E_F \in \mathbb{R}$ and $m \geqslant 0$ such that $E_F > m$. Then we have*

$$\begin{aligned}&\frac{2}{n}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[h\Big(\mathbf{1}_\Omega \operatorname{Op}_L\big(\chi^{(b)}_{E_F}(D)\big)\mathbf{1}_\Omega\Big)\Big]\\ &\quad= L^d V_+(h, b, E_F, m)|\Omega| + L^{d-1}\log L\ W(h, \Omega, E_F, m) + o(L^{d-1}\log L),\end{aligned} \tag{5.29}$$

as $L \to \infty$, where

$$V_+(h, b, E_F, m) := V_-(h, b, E_F, m) + \frac{2|B_{p_F}|}{(2\pi)^d}\,h(1) \tag{5.30}$$

is independent of n and Ω.

Proof. In the case $E_F > m$ we obtain $\big(\chi_{E_F}^{(b)}\big)_+(\xi) = 1_\Gamma(\xi)$ and $\big(\chi_{E_F}^{(b)}\big)_-(\xi) = \varphi(-E(\xi)+b) = \tilde{\varphi}^{(b)}(\xi)$ for the functions from (5.13). Further, we have $\big(\chi_{E_F}^{(b)}\big)_-|_\Gamma = 1$ by the definition of $\tilde{\varphi}^{(b)}$. Therefore, we can write $\big(\chi_{E_F}^{(b)}\big)_-(\xi) = 1_\Gamma(\xi) + 1_{\Gamma^c}(\xi)\tilde{\varphi}^{(b)}(\xi)$. Applying (5.13), the operator in question reads

$$\begin{aligned} &h\big(\mathbf{1}_\Omega \operatorname{Op}_L(\chi_{E_F}^{(b)}(D))\mathbf{1}_\Omega\big) \\ &\qquad = h\Big(\mathbf{1}_\Omega\big\{\operatorname{Op}_L(\mathbf{1}_\Gamma) + \operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\operatorname{Op}_L\big(\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big)\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\big\}\mathbf{1}_\Omega\Big). \end{aligned} \tag{5.31}$$

As in the proof of Lemma 5.3, after (5.18), we can replace the function $\tilde{\varphi}^{(b)}$ in (5.31) by a function $\varphi^{(b)} \in C_c^\infty(\mathbb{R}^d)$ with $\varphi^{(b)}(0) = 0$ without changing the result. This guarantees that the symbols $A_1 := \mathbb{1}_n$ and $A_2 := \frac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \frac{D}{E})$ are smooth, bounded and the latter also compactly supported. Thus, we can apply Theorem 4.29 with the symbols A_1 and A_2 as above. This yields the asymptotic expansion

$$\begin{aligned} &\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[h\Big(\mathbf{1}_\Omega\big\{\operatorname{Op}_L(\mathbf{1}_\Gamma) + \operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\operatorname{Op}_L\big(\tfrac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big)\operatorname{Op}_L(\mathbf{1}_{\Gamma^c})\big\}\mathbf{1}_\Omega\Big)\Big] \\ &\quad = L^d\,\mathfrak{W}_0\Big(\operatorname{tr}_{\mathbb{C}^n}\big[h(\mathbb{1}_n)\big];\Omega,\Gamma\Big) \\ &\qquad + L^d\,\mathfrak{W}_0\Big(\operatorname{tr}_{\mathbb{C}^n}\big[h\big(\tfrac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big)\big];\Omega,\Gamma^c\Big) \\ &\qquad + L^{d-1}\log L\,\mathfrak{W}_1\Big(\mathfrak{U}\big(h;\mathbb{1}_n,\tfrac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big);\partial\Omega,\partial\Gamma\Big) \\ &\qquad + o(L^{d-1}\log L), \end{aligned} \tag{5.32}$$

as $L \to \infty$. We observe

$$\operatorname{tr}_{\mathbb{C}^n}[h(\mathbb{1}_n)] = nh(1) \tag{5.33}$$

and claim

$$\begin{aligned} &\mathfrak{W}_0\Big(\operatorname{tr}_{\mathbb{C}^n}\big[h(\mathbb{1}_n)\big];\Omega,\Gamma\Big) + \mathfrak{W}_0\Big(\operatorname{tr}_{\mathbb{C}^n}\big[h\big(\tfrac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big)\big];\Omega,\Gamma^c\Big) \\ &\qquad = \frac{n}{2}\,|\Omega|\left[\frac{2|\Gamma|}{(2\pi)^d}\,h(1) + V_-(h,b,E_F,m)\right]. \end{aligned} \tag{5.34}$$

Here, the first coefficient was evaluated with the definition (5.20) and the second one with the identity (5.27).

In order to treat the coefficient of the enhanced area term, we observe that by argument-wise diagonalisation, $\frac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \frac{D}{E}) = \frac{1}{2}U^{-1}\varphi^{(b)}(\mathbb{1}_n - \beta)U$ as in (2.42), we obtain for all $\xi \in \partial\Gamma$, for which $\varphi^{(b)}(\xi) = 1$,

$$\begin{aligned} &\operatorname{tr}_{\mathbb{C}^n}\Big[h\Big(\mathbb{1}_n t + \tfrac{1}{2}\varphi^{(b)}(\xi)\big(\mathbb{1}_n - \tfrac{D}{E}(\xi)\big)(1-t)\Big)\Big] \\ &\qquad = \operatorname{tr}_{\mathbb{C}^n}\Big[U^{-1}(\xi)h\Big(\mathbb{1}_n t + \tfrac{1}{2}(\mathbb{1}_n - \beta)(1-t)\Big)U(\xi)\Big] \\ &\qquad = \operatorname{tr}_{\mathbb{C}^n}\begin{pmatrix} h(t)\mathbb{1}_{\frac{n}{2}} & 0 \\ 0 & h(1)\mathbb{1}_{\frac{n}{2}} \end{pmatrix} = \frac{n}{2}\,[h(t) + h(1)]. \end{aligned} \tag{5.35}$$

Using this identity, (5.33) and (5.24) with $z = 1$ and $\varphi^{(b)} = 1$, we obtain from the definition (5.23)

$$\begin{aligned}
&\mathfrak{U}\big(h; \mathbb{1}_n, \tfrac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big)(\xi)\\
&\quad = \frac{1}{(2\pi)^2}\int_0^1 \frac{1}{t(1-t)}\operatorname{tr}_{\mathbb{C}^n}\Big[h\Big(\mathbb{1}_n t + \tfrac{1}{2}\varphi^{(b)}(\xi)\big(\mathbb{1}_n - \tfrac{D}{E}(\xi)\big)(1-t)\Big)\\
&\qquad\qquad - h(\mathbb{1}_n)t - h\Big(\tfrac{1}{2}\varphi^{(b)}(\xi)\big(\mathbb{1}_n - \tfrac{D}{E}(\xi)\big)\Big)(1-t)\Big]\,\mathrm{d}t\\
&\quad = \frac{n}{2}\frac{1}{(2\pi)^2}\int_0^1 \frac{h(t) + h(1) - 2h(1)t - h(1)(1-t)}{t(1-t)}\,\mathrm{d}t\\
&\quad = \frac{n}{2}\,\mathfrak{A}(h;1),
\end{aligned} \tag{5.36}$$

where we refer to (5.26) for the symbol $\mathfrak{A}$. Accordingly, the symbol (5.36) is constant on $\partial\Gamma$, and the relation (5.22) yields

$$\begin{aligned}
\mathfrak{W}_1\Big(\mathfrak{U}\big(h; \mathbb{1}_n, \tfrac{1}{2}\varphi^{(b)}(\mathbb{1}_n - \tfrac{D}{E})\big); \partial\Omega, \partial\Gamma\Big) &= \frac{n}{2}\frac{1}{(2\pi)^2}\int_0^1 \frac{h(t) - h(1)}{t(1-t)}\,\mathrm{d}t\;\Phi(\Omega, E_F, m)\\
&= \frac{n}{2}\,W(h, \Omega, E_F, m).
\end{aligned} \tag{5.37}$$

Therefore, the claim follows from (5.37), (5.34), (5.32) and (5.31). □

5.3. The case $|E_F| \leqslant m \neq 0$

The key observation in this case is that the discontinuity of the function $\chi_{E_F}^{(b)}$ does not affect the symbol $\chi_{E_F}^{(b)}(D)$. This is because there exists a function $\tilde{\chi}_{E_F}^{(b)} \in C_c^\infty(\mathbb{R})$ with $\operatorname{supp}\big(\chi_{E_F}^{(b)} - \tilde{\chi}_{E_F}^{(b)}\big) \subseteq [-m, m]$. Therefore, Remark 2.10(d) allows us to replace $\chi_{E_F}^{(b)}$ by $\tilde{\chi}_{E_F}^{(b)}$ without changing the symbol, $\tilde{\chi}_{E_F}^{(b)}(D) = \chi_{E_F}^{(b)}(D)$ Lebesgue-a.e., and Remark 2.10(e) guarantees smoothness of the symbol $\tilde{\chi}_{E_F}^{(b)}(D)$. We now show that this is sufficient to obtain the desired estimate for (5.14) from Lemmas 3.6 and 4.26.

Lemma 5.5. *Let h be as in Theorem 5.1, Ω be a bounded admissible domain, $b \geqslant 0$, $E_F \in \mathbb{R}$ and $m > 0$ such that $|E_F| \leqslant m$. Then, for every $L \geqslant 1$, we have*

$$\Big\| h\Big(\mathbf{1}_\Omega \operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_\Omega\Big) - \mathbf{1}_\Omega \operatorname{Op}_L\Big(h\big(\chi_{E_F}^{(b)}(D)\big)\Big)\mathbf{1}_\Omega\Big\|_1 \leqslant C L^{d-1}, \tag{5.38}$$

where the constant $C > 0$ is independent of L.

Proof. As $\chi_{E_F}^{(b)}$ and thus the operator $\operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)$ is bounded, we can assume that the function h is compactly supported. An application of Lemma 4.26, with $A = \operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)$, $P = \mathbf{1}_\Omega$ and arbitrary $q \in]0, \gamma[$, yields

$$\Big\| h\Big(\mathbf{1}_\Omega \operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_\Omega\Big) - \mathbf{1}_\Omega \operatorname{Op}_L\Big(h\big(\chi_{E_F}^{(b)}(D)\big)\Big)\mathbf{1}_\Omega\Big\|_1 \leqslant C_1 \big\|\mathbf{1}_\Omega \operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_{\Omega^c}\big\|_q^q, \tag{5.39}$$

where the constant $C_1 > 0$ does not depend on the parameter L. Therefore, it suffices to show

$$\big\|\mathbf{1}_\Omega \operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_{\Omega^c}\big\|_q^q \leqslant C_2 L^{d-1} \tag{5.40}$$

for some constant $C_2 > 0$ which does not depend on L. As discussed at the beginning of this section, we can replace the discontinuous symbol $\chi_{E_F}^{(b)}(D)$ by $\tilde{\chi}_{E_F}^{(b)}(D) \in C_c^\infty(\mathbb{R}^d)$. As Ω is bounded, there exists a function $\phi \in C_c^\infty(\mathbb{R}^d)$ with $\phi|_\Omega = 1$, and we have $\phi\tilde{\chi}_{E_F}^{(b)}(D) \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$. As Ω is also admissible, we can apply Lemma 3.6 with $A = \phi\tilde{\chi}_{E_F}^{(b)}(D)$ and $\Lambda = \Omega$ to obtain the desired result. □

5.4. The case $E_F = m = 0$

If $|E_F| = m = 0$, we obtain the functions $\big(\chi_0^{(b)}\big)_+ = 0$ and $\big(\chi_0^{(b)}\big)_- = 1_{\{y\in\mathbb{R}:\, y<0\}}(-E)\varphi(-E+b) = 1_{\mathbb{R}^d\setminus\{0\}}\varphi(-E+b)$. As in the proof of Lemma 5.3 we define the function $\tilde{\varphi}^{(b)}$ by $\tilde{\varphi}^{(b)}(\xi) := \varphi(-E(\xi)+b)$ for every $\xi \in \mathbb{R}^d$. It only differs from $\big(\chi_0^{(b)}\big)_-$ at the origin $\xi = 0$, i.e. on a set of Lebesgue measure zero. Therefore, after an application of (5.13), the relevant operator reads

$$\mathbf{1}_\Omega \operatorname{Op}_L\big(\chi_0^{(b)}(D)\big)\mathbf{1}_\Omega = \mathbf{1}_\Omega \operatorname{Op}_L\Big(\tfrac{1}{2}\tilde{\varphi}^{(b)}\big(\mathbb{1}_n - \tfrac{D}{E}\big)\Big)\mathbf{1}_\Omega. \tag{5.41}$$

We observe that the symbol $\frac{1}{2}\tilde{\varphi}^{(b)}\big(\mathbb{1}_n - \frac{D}{E}\big) \in C_c^\infty(\mathbb{R}^d \setminus \{0\})$ has a discontinuity at the origin. It will turn out that this zero-dimensional discontinuity leads to the same behaviour as in Section 5.2 in dimension one. In higher dimensions, it will lead to the same behaviour as in Section 5.3.

We will first consider the case $d = 1$, where, accordingly $n = n_1 = 2$.

Lemma 5.6. *Let h be as in Theorem 5.1, Ω be a bounded piece-wise C^1-admissible domain, $b \geqslant 0$, $E_F = m = 0$ and $d = 1$. Then we have*

$$\frac{2}{n}\operatorname{tr}_{L^2(\mathbb{R})\otimes\mathbb{C}^2}\Big[h\Big(\mathbf{1}_\Omega \operatorname{Op}_L\big(\chi_0^{(b)}(D)\big)\mathbf{1}_\Omega\Big)\Big] = LV_0(h,b)|\Omega| + \log L\, W(h,\Omega,0,0) + o(\log L), \tag{5.42}$$

as $L \to \infty$, where

$$V_0(h,b) := \frac{1}{2\pi}\int_{\mathbb{R}} \big[h \circ \big(\chi_0^{(b)}\big)_-\big](\xi)\,\mathrm{d}\xi \tag{5.43}$$

is independent of Ω.

Proof. If $d = 1$ and $m = 0$, there is only one relevant Dirac matrix. We choose

$$D(\xi) = \sum_{k=1}^{1}\alpha_k\xi_k + m\beta = \alpha_1\xi = \begin{pmatrix} 0 & \xi \\ \xi & 0 \end{pmatrix}. \tag{5.44}$$

We define the (unbounded) admissible domain $\Gamma :=]-\infty, 0[$ and write

$$\mathbb{1}_2 - \frac{D}{E} = \begin{pmatrix} 1 & -\operatorname{sgn} \\ -\operatorname{sgn} & 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\mathbf{1}_\Gamma + \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}\mathbf{1}_{\Gamma^c} = (\mathbb{1}_2 + \alpha_1)\mathbf{1}_\Gamma + (\mathbb{1}_2 - \alpha_1)\mathbf{1}_{\Gamma^c}, \tag{5.45}$$

where the second equality holds for all $\xi \in \mathbb{R} \setminus \{0\}$, as we use the conventions $\frac{D}{E}(0) = 0$ and $\operatorname{sgn}(0) = 0$ for the sign function sgn on $\mathbb{R}$. With this, the operator on the right-hand side of (5.41) reads

$$\mathbf{1}_\Omega\Big[\operatorname{Op}_L\Big(\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2 + \alpha_1)\mathbf{1}_\Gamma\Big) + \operatorname{Op}_L\Big(\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2 - \alpha_1)\mathbf{1}_{\Gamma^c}\Big)\Big]\mathbf{1}_\Omega. \tag{5.46}$$

We note that the symbol $\tilde{\varphi}^{(b)}$ is smooth, bounded and compactly supported. Therefore, the symbols $A_1 := \frac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2 + \alpha_1)$ and $A_2 := \frac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2 - \alpha_1)$ are also smooth, bounded and compactly supported.

An application of Theorem 4.29, Remark 4.30 yields the asymptotic expansion

$$\begin{aligned}
&\operatorname{tr}_{L^2(\mathbb{R})\otimes\mathbb{C}^2}\Big[h\Big(\mathbf{1}_\Omega \operatorname{Op}_L\Big(\tfrac{1}{2}\tilde{\varphi}^{(b)}\big((\mathbb{1}_2+\alpha_1)\mathbf{1}_\Gamma+(\mathbb{1}_2-\alpha_1)\mathbf{1}_{\Gamma^c}\big)\Big)\mathbf{1}_\Omega\Big)\Big]\\
&\qquad= L\,\mathfrak{W}_0\Big(\operatorname{tr}_{\mathbb{C}^2}\big[h\big(\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2+\alpha_1)\big)\big];\Omega,\Gamma\Big)\\
&\qquad\quad+ L\,\mathfrak{W}_0\Big(\operatorname{tr}_{\mathbb{C}^2}\big[h\big(\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2-\alpha_1)\big)\big];\Omega,\Gamma^c\Big)\\
&\qquad\quad+\log L\,\mathfrak{W}_1\Big(\mathfrak{U}\big(h;\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2+\alpha_1),\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2-\alpha_1)\big);\partial\Omega,\partial\Gamma\Big)\\
&\qquad\quad+o(\log L),
\end{aligned}\tag{5.47}$$

as $L\to\infty$. We infer from the eigenvalues of the matrices $\mathbb{1}_2+\alpha_1$, $\mathbb{1}_2-\alpha_1$ and $\mathbb{1}_2+(2t-1)\alpha_1$ that

$$\operatorname{tr}_{\mathbb{C}^2}\big[h\big(\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2+\alpha_1)\big)\big]=h(\tilde{\varphi}^{(b)})=\operatorname{tr}_{\mathbb{C}^2}\big[h\big(\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2-\alpha_1)\big)\big]\tag{5.48}$$

and

$$\operatorname{tr}_{\mathbb{C}^2}\big[h\big(\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2+\alpha_1)t+\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2-\alpha_1)(1-t)\big)\big]=h\big(\tilde{\varphi}^{(b)}t\big)+h\big(\tilde{\varphi}^{(b)}(1-t)\big),\tag{5.49}$$

so that

$$\begin{aligned}
&\mathfrak{U}\Big(h;\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2+\alpha_1),\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2-\alpha_1)\Big)\\
&\quad=\frac{1}{(2\pi)^2}\int_0^1\frac{h\big(\tilde{\varphi}^{(b)}t\big)+h\big(\tilde{\varphi}^{(b)}(1-t)\big)-h\big(\tilde{\varphi}^{(b)}\big)t-h\big(\tilde{\varphi}^{(b)}\big)(1-t)}{t(1-t)}\,\mathrm{d}t\\
&\quad=2\,\mathfrak{A}\big(h;\tilde{\varphi}^{(b)}\big).
\end{aligned}\tag{5.50}$$

Thus, we obtain the volume coefficient

$$\begin{aligned}
&\mathfrak{W}_0\Big(\operatorname{tr}_{\mathbb{C}^2}\big[h\big(\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2+\alpha_1)\big)\big];\Omega,\Gamma\Big)+\mathfrak{W}_0\Big(\operatorname{tr}_{\mathbb{C}^2}\big[h\big(\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2-\alpha_1)\big)\big];\Omega,\Gamma^c\Big)\\
&\qquad=\frac{|\Omega|}{2\pi}\int_{\mathbb{R}}\big(h(\tilde{\varphi}^{(b)})\big)(\xi)\,\mathrm{d}\xi=|\Omega|V_0(h,b)
\end{aligned}\tag{5.51}$$

and the coefficient of the enhanced area term

$$\begin{aligned}
&\mathfrak{W}_1\Big(\mathfrak{U}\big(h;\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2+\alpha_1),\tfrac{1}{2}\tilde{\varphi}^{(b)}(\mathbb{1}_2-\alpha_1)\big);\partial\Omega,\partial\Gamma\Big)=2\,\mathfrak{W}_1\big(\mathfrak{A}\big(h;\tilde{\varphi}^{(b)}\big);\partial\Omega,\partial\Gamma\big)\\
&\qquad=\frac{\Phi(\Omega,0,0)}{(2\pi)^2}\int_0^1\frac{h(t)-h(1)t}{t(1-t)}\mathrm{d}t\;=W(h,\Omega,0,0),
\end{aligned}\tag{5.52}$$

where we used (5.22) together with $\tilde{\varphi}^{(b)}|_{\partial\Gamma}=\tilde{\varphi}^{(b)}(0)=1$ for the second equality. Now, the lemma follows from (5.52), (5.51), (5.47) and (5.46). □

Remark 5.7. Upon comparing the proof of Lemma 5.6 with the proofs of Lemma 5.3 and 5.4 in $d=1$ and recalling $n=n_1=2$, we observe an additional factor of 2 in (5.50) as compared to (5.25) or (5.36). On the other hand, we have $|\partial\Gamma|=1$ in the proof of Lemma 5.6, whereas $|\partial\Gamma|=2$ in the proofs of Lemma 5.3 and 5.4. Still, this allows to write the coefficient of the enhanced area term in Lemma 5.6 in the same way as in Lemma 5.3 and 5.4 by attributing the additional factor of 2 from (5.50) to the geometric factor $\Phi(\Omega,0,0)$ in the second equality of (5.52).

Next, we consider the higher-dimensional case. Here we want to show that the discontinuity at the origin does not alter the situation in Section 5.3. We proceed as in Section 5.3 and apply Lemma 4.26. The difference is the estimate for the Schatten–von Neumann norm, as the result used in the Section 5.3 requires a smooth symbol and therefore does not apply now. Instead we apply the Schatten–von Neumann estimate for symbols which are discontinuous at the origin, obtained in

Chapter 3. A related estimate was recently obtained in [FLS24, Lemma 4.3]. Both estimates were obtained independently of one another.

With this, the desired estimate then follows immediately.

Lemma 5.8. *Let h be as in Theorem 5.1, Ω be a bounded admissible domain, $b \geqslant 0$, $E_F = m = 0$ and $d \geqslant 2$. Then, for every $L \geqslant 2$, we have*

$$\Big\| h\Big(\mathbf{1}_\Omega \operatorname{Op}_L\big(\chi_0^{(b)}(D)\big)\mathbf{1}_\Omega\Big) - \mathbf{1}_\Omega \operatorname{Op}_L\Big(h\big(\chi_0^{(b)}(D)\big)\Big)\mathbf{1}_\Omega\Big\|_1 \leqslant C L^{d-1}, \tag{5.53}$$

where the constant $C > 0$ is independent of L.

Proof. As $\chi_0^{(b)}$ and thus the operator $\operatorname{Op}_L\big(\chi_0^{(b)}(D)\big)$ is bounded, we can assume that the function h is compactly supported. An application of Lemma 4.26 with $A = \operatorname{Op}_L\big(\chi_0^{(b)}(D)\big)$, $P = \mathbf{1}_\Omega$ and arbitrary $q \in]0,\gamma[$ yields

$$\Big\| h\Big(\mathbf{1}_\Omega \operatorname{Op}_L\big(\chi_0^{(b)}(D)\big)\mathbf{1}_\Omega\Big) - \mathbf{1}_\Omega \operatorname{Op}_L\Big(h\big(\chi_0^{(b)}(D)\big)\Big)\mathbf{1}_\Omega\Big\|_1 \leqslant C_1 \Big\|\mathbf{1}_\Omega \operatorname{Op}_L\big(\chi_0^{(b)}(D)\big)\mathbf{1}_{\Omega^c}\Big\|_q^q, \tag{5.54}$$

where the constant $C_1 > 0$ does not depend on the parameter L. Therefore, the claim follows from an application of Lemma 3.9 in the case $d \geqslant 2$. □

5.5. Proof of the main result

All that remains to be done is to collect the previous statements.

Proof of Theorem 5.1. For fixed $L > 0$ we rewrite the left-hand side of (5.4) as

$$\frac{1}{n}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[h\Big(\mathbf{1}_\Lambda \operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_\Lambda\Big) \\ + h\Big(\mathbf{1}_{\Lambda'\setminus\Lambda} \operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_{\Lambda'\setminus\Lambda}\Big) - h\Big(\mathbf{1}_{\Lambda'} \operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_{\Lambda'}\Big)\Big] \tag{5.55}$$

by (5.9) and (5.11). As both Λ and Λ' are bounded piece-wise C^1-admissible domains, the domain $\Lambda' \setminus \Lambda$ is also a bounded piece-wise C^1-admissible domain up to a set of measure zero.

Firstly, we treat the situations where there will be a logarithmic enhancement. So, we consider either the case $|E_F| > m$ or the case $E_F = m = 0$ in $d = 1$. In order to cover these simultaneously, we introduce the asymptotic volume coefficient

$$V(h,b,E_F,m) := \begin{cases} V_-(h,b,E_F,m), & \text{if } E_F < -m, \\ V_+(h,b,E_F,m), & \text{if } E_F > m, \\ V_0(h,b), & \text{if } E_F = m = 0 \text{ and } d = 1. \end{cases} \tag{5.56}$$

In the first case, we apply Lemma 5.3, in the second case Lemma 5.4 and in the third case Lemma 5.6 to all three terms in (5.55). This yields the asymptotic expansion

$$\frac{1}{2} L^d V(h,b,E_F,m)\Big(|\Lambda| + |\Lambda'\setminus\Lambda| - |\Lambda'|\Big) \\ + \frac{1}{2} L^{d-1}\log L\Big(W(h,\Lambda,E_F,m) + W(h,\Lambda'\setminus\Lambda,E_F,m) - W(h,\Lambda',E_F,m)\Big) + o(L^{d-1}\log L) \tag{5.57}$$

of (5.55), as $L \to \infty$. Now, the volumes in the first line of (5.57) add up to zero, and by the definition of $W(h,\Lambda,E_F,m)$ in Theorem 5.1 we have

$$W(h,\Lambda,E_F,m) + W(h,\Lambda'\setminus\Lambda,E_F,m) - W(h,\Lambda',E_F,m) = 2W(h,\Lambda,E_F,m). \tag{5.58}$$

Thus, we infer the desired result

$$\begin{aligned}\frac{1}{n}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[h\big(\mathbf{1}_{\Lambda_L}\chi_{E_F}^{(b)}(D)\mathbf{1}_{\Lambda_L}\big)+h\big(\mathbf{1}_{\Lambda'_L\setminus\Lambda_L}\chi_{E_F}^{(b)}(D)\mathbf{1}_{\Lambda'_L\setminus\Lambda_L}\big)-h\big(\mathbf{1}_{\Lambda'_L}\chi_{E_F}^{(b)}(D)\mathbf{1}_{\Lambda'_L}\big)\Big]&\\ = L^{d-1}\log L\;W(h,\Lambda,E_F,m)+o(L^{d-1}\log L),&\quad (5.59)\end{aligned}$$

as $L\to\infty$.

Secondly, we turn to the situations without logarithmic enhancement, that is, the case $|E_F|\leqslant m\neq 0$ and the case $E_F=m=0$ in $d\geqslant 2$. We observe that for fixed $L>0$ we have

$$\begin{aligned}\mathbf{1}_\Lambda\operatorname{Op}_L\Big(h\big(\chi_{E_F}^{(b)}(D)\big)\Big)\mathbf{1}_\Lambda+\mathbf{1}_{\Lambda'\setminus\Lambda}\operatorname{Op}_L\Big(h\big(\chi_{E_F}^{(b)}(D)\big)\Big)\mathbf{1}_{\Lambda'\setminus\Lambda}-\mathbf{1}_{\Lambda'}\operatorname{Op}_L\Big(h\big(\chi_{E_F}^{(b)}(D)\big)\Big)\mathbf{1}_{\Lambda'}&\\ =-\mathbf{1}_\Lambda\operatorname{Op}_L\Big(h\big(\chi_{E_F}^{(b)}(D)\big)\Big)\mathbf{1}_{\Lambda'\setminus\Lambda}-\mathbf{1}_{\Lambda'\setminus\Lambda}\operatorname{Op}_L\Big(h\big(\chi_{E_F}^{(b)}(D)\big)\Big)\mathbf{1}_\Lambda.&\quad (5.60)\end{aligned}$$

Both operators in the last line of (5.60) have vanishing trace. Therefore, we can rewrite (5.55) as

$$\begin{aligned}\frac{1}{n}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[&h\Big(\mathbf{1}_\Lambda\operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_\Lambda\Big)-\mathbf{1}_\Lambda\operatorname{Op}_L\Big(h\big(\chi_{E_F}^{(b)}(D)\big)\Big)\mathbf{1}_\Lambda\\ &+h\Big(\mathbf{1}_{\Lambda'\setminus\Lambda}\operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_{\Lambda'\setminus\Lambda}\Big)-\mathbf{1}_{\Lambda'\setminus\Lambda}\operatorname{Op}_L\Big(h\big(\chi_{E_F}^{(b)}(D)\big)\Big)\mathbf{1}_{\Lambda'\setminus\Lambda}\\ &-h\Big(\mathbf{1}_{\Lambda'}\operatorname{Op}_L\big(\chi_{E_F}^{(b)}(D)\big)\mathbf{1}_{\Lambda'}\Big)+\mathbf{1}_{\Lambda'}\operatorname{Op}_L\Big(h\big(\chi_{E_F}^{(b)}(D)\big)\Big)\mathbf{1}_{\Lambda'}\Big]\qquad (5.61)\end{aligned}$$

and estimate the trace norm of the operator difference in each of the three lines by Lemma 5.5 in the case $|E_F|\leqslant m\neq 0$ and by Lemma 5.8 in the case $E_F=m=0$ and $d\geqslant 2$. This yields the existence of a constant $C>0$ such that the modulus of (5.61) is bounded from above by CL^{d-1} for all $L\geqslant 2$, and the proof is complete. □

CHAPTER 6

An enhanced term of lower order in the massless case

Context: The majority of this chapter coincides, in both content and writing, with [Bol25]. Some of the proofs have been extended. A simplified overview of the proof's strategy (which is not present in [Bol25]) has been included in Section 6.2.

Content: In this chapter we study the lower-order terms of the asymptotic expansion for the free Dirac operator in the massless case. In Section 6.1 we recall the symbol of the free massless Dirac operator, state our main results and discuss these results and the required assumptions on both cut-off domains and test functions. In Section 6.2 we take a closer look at the decay of the integral kernel of the operator and give an overview of the strategy of the proof. In Section 6.3 we utilise the obtained decay estimates for the integral kernel to obtain the first d terms of the asymptotic expansion and to localise the operator remaining after subtraction of these first d terms. Section 6.4 begins with some additional estimates for pseudo-differential operators with smooth symbols. Utilising these estimates, we find a logarithmic upper bound for the remaining operator from Section 6.3. In Section 6.5 we further analyse this remaining term. Using the structure of this term and the estimates for smooth symbols from Section 6.4, we commute all occurrences of the smooth regularisation of the Fermi projection to one side of the operator, up to error terms of constant order. The last Section 6.6 consists of two parts: In the first part we derive certain properties for the operator obtained through the commutation in Section 6.5. We only do this for polynomial test functions of degree three or less. The second part consists of a local asymptotic formula under the assumptions that the properties derived in the first part hold. With this and the results from the previous sections, we obtain a $(d+1)$-term asymptotic expansion, with the last term being of logarithmic order and independent of the smooth regularisation of the Fermi projection.

6.1. Discussion of results

We stick to the notation introduced in Chapter 2. As the one-dimensional case is already discussed in Chapter 5, we restrict ourselves to the case $d \geqslant 2$. The goal of the present chapter is to further investigate the lower-order terms in the Szegő-type asymptotic expansion of the massless Dirac-operator. We recall that the symbol obtained by applying the smoothly regularised Fermi projection $\chi_0^{(b)}$ at Fermi energy zero to the massless Dirac operator is given by

$$\big(\chi_0^{(b)}(D)\big)(\xi) = \psi^{(b)}(\xi)\tfrac{1}{2}\big(\mathbb{1}_n - \tfrac{D}{E}(\xi)\big) = \psi^{(b)}(\xi)\tfrac{1}{2}\Big(\mathbb{1}_n - \sum_{k=1}^{d} \alpha_k \tfrac{\xi_k}{|\xi|}\Big) =: \psi^{(b)}(\xi)\mathcal{D}(\xi), \tag{6.1}$$

where we use the convention $\frac{D}{E}(0) = 0$ and $\psi(\xi) := \psi^{(b)}(\xi) := \varphi(-E(\xi) + b)$ for every $\xi \in \mathbb{R}^d$, with φ being defined in (2.43) and E being the energy given by $E(\xi) = |\xi|$ for $\xi \in \mathbb{R}^d$. The symbol $\psi^{(b)}$ is smooth and compactly supported in the ball $B_{b+1}(0)$ of radius $b+1$ centred about the origin, and satisfies $\|\psi^{(b)}\|_\infty = 1$. It will be notationally convenient to drop the superscript (b) of the symbol

ψ beginning with Section 6.2 of the present chapter. The symbol $\mathcal{D}$ features a zero-dimensional discontinuity at the origin and is smooth everywhere else.

In Theorem 5.1 we proved that the zero-dimensional discontinuity of this symbol yields a logarithmically enhanced area law in dimension one. In higher dimensions we proved that not more than an area law can hold. As the leading and subleading terms of the expansion are of the same order as the corresponding terms for continuous symbols in this case, we now want to study the expansion beyond the subleading term in order to discern the effect the zero-dimensional discontinuity has on the expansion. The one-dimensional case suggests a lower-order logarithmically enhanced term of order $\log L$, and, in analogy to the interaction of the two $(d-1)$-dimensional boundaries $\partial\Lambda$ and $\partial\Gamma$ in the enhanced area coefficient of the Widom–Sobolev formula, one might expect an interaction of the zero-dimensional discontinuity with zero-dimensional points in the boundary of Λ, where the smoothness of the boundary breaks down, e.g. the vertices of a d-dimensional cube. In the next section we also take a different perspective on the symbol which supports the idea of a lower-order term of logarithmic order. As we will see, the off-diagonal decay of the integral kernel corresponding to the symbol is of order $|x-y|^{-d}$. Comparing this decay with the decay of order $|x-y|^{-(d+1)/2}$, required to obtain the subleading term in [Wid80], suggests that even the first d terms of the asymptotic expansion are of the same order as in the case with continuous symbol, and only starting with the $(d+1)$st term the order of the terms changes.

The aforementioned suspected interaction with vertices guides our choice of spatial cut-off domains in the sense that we are especially interested in studying domains Λ with only piece-wise smooth boundary. Our choice are d-dimensional cubes, as they still have a sufficiently simple structure in higher dimensions, which helps us illustrate the general structure of the asymptotic expansion depending on the dimension d. Furthermore, we can use the already established $(d+1)$-term expansions for cubes in the case with continuous symbol [Die18] as a starting point. For convenience we choose the cubes $\Lambda = [0,2]^d$. The expansion for more general cubes $[0,2a]^d + b$, for $a > 0$, $b \in \mathbb{R}^d$, follows easily by the translation invariance of $\mathrm{Op}(\psi^{(b)}\mathcal{D})$ and a change of scaling parameter $L \mapsto aL$.

The structure of the cube Λ is also responsible for the structure of the coefficients of the first d terms of the asymptotic expansion. For $m \in \{0,\dots,d-1\}$ and a suitable test function $h : \mathbb{C} \to \mathbb{C}$ with $h(0)$, the coefficient of the term of order L^{d-m} is given by

$$A_{m,h,b} := \lim_{L\to\infty} \mathrm{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \left[\sum_{k=0}^{m} c_{k,m} \mathbf{1}_{[0,L]^m\times[0,1]^{d-m}} h\big(X_{m,k,b}\big) \right], \tag{6.2}$$

where we used the abbreviation $X_{m,k,b} := \mathbf{1}_{\mathbb{R}_+^{m-k}\times\mathbb{R}^{d-m+k}} \mathrm{Op}(\psi^{(b)}\mathcal{D}) \mathbf{1}_{\mathbb{R}_+^{m-k}\times\mathbb{R}^{d-m+k}}$ and the constants $c_{k,m}$ are given by $c_{k,m} := \frac{(-1)^k 2^m d!}{k!(m-k)!(d-m)!}$ for $0 \leqslant k \leqslant m \leqslant d-1$. We will see in Section 6.3 that these coefficients are actually well-defined. We note that the limits of the individual operators in the trace in (6.2) are not trace class and therefore the limit can not be interchanged with the trace. We further note that the index $m \in \{0,\dots,d-1\}$ is not to be confused with the physical mass introduced in Section 2.2 which is always assumed to be zero in the present chapter. Although it would certainly be desirable to obtain the asymptotic expansion for the class of test functions satisfying Assumption 2.5, the structure of these coefficients already illustrates why we restrict ourselves to analytic test functions instead. For the sake of this illustration, we assume that we are in dimension $d = 3$. For the subleading term, i.e. in the case $m = 1$, the coefficient stems from the following operator difference corresponding to the approximation of the cube by one of its 2-dimensional faces

$$\mathbf{1}_{[0,L]^3}\big[h\big(\mathbf{1}_{\mathbb{R}_+\times\mathbb{R}^2} \mathrm{Op}(\psi^{(b)}\mathcal{D})\mathbf{1}_{\mathbb{R}_+\times\mathbb{R}^2}\big) - h\big(\mathrm{Op}(\psi^{(b)}\mathcal{D})\big)\big]\mathbf{1}_{[0,L]^3}. \tag{6.3}$$

Using the abbreviations $P = \mathbf{1}_{[0,\infty[\times\mathbb{R}^2}$, $Q = \mathbf{1}_{[0,L]^3}$ and $A = \mathrm{Op}(\psi^{(b)}\mathcal{D})$, as well as the fact that Q is a projection, we see that this difference has the structure

$$h(PAP)Q - Qh(A). \tag{6.4}$$

The analysis of such "quasi-commutators" in [Sob17] is the basis for studying test functions satisfying Assumption 2.5, cf. the proofs in Section 4.6. Using [Sob17, Thm. 2.4] and the fact that $QP = Q$, we see that the trace norm of (6.4) is bounded by a constant times the following Schatten–von Neumann norm

$$\|PAQ - QA\|_q^q \leqslant \|(P-Q)AQ\|_q^q + \|QA(1-Q)\|_q^q, \tag{6.5}$$

for a suitable $q \in]0,1[$ depending on h. An application of Lemma 3.9 then yields that both the terms on the right-hand side of (6.5) are of order L^2. For the term of order L, i.e. in the case $m = 2$, the situation is more complicated, as we also need to consider the operator difference

$$\mathbf{1}_{[0,L]^3}\big[h\big(\mathbf{1}_{\mathbb{R}_+^2\times\mathbb{R}}\,\mathrm{Op}(\psi^{(b)}\mathcal{D})\mathbf{1}_{\mathbb{R}_+^2\times\mathbb{R}}\big) - h\big(\mathbf{1}_{\mathbb{R}_+\times\mathbb{R}^2}\,\mathrm{Op}(\psi^{(b)}\mathcal{D})\mathbf{1}_{\mathbb{R}_+\times\mathbb{R}^2}\big)\big]\mathbf{1}_{[0,L]^3}. \tag{6.6}$$

For suitable projections P, P' and Q, this is of the form

$$h(PAP)Q - Qh(P'AP') \tag{6.7}$$

and we can use the same strategy as before to reduce this to the bound

$$\|PAQ - QAP'\|_q^q \leqslant \|(P-Q)AQ\|_q^q + \|QA(P'-Q)\|_q^q. \tag{6.8}$$

We again see that this is of order L^2, but as we now study the term of order L, this bound is not sufficient. As this blocks the usual route of closing the asymptotics for these more general functions as in Section 4.6, one would require a different approach which makes use of the projections on both sides of (6.6), instead of using the "quasi-commutator" structure as in [Sob17, Thm. 2.4]. Unfortunately, the compatibility of the "quasi-commutator" structure and the second resolvent identity seems to be integral for the proof of [Sob17, Thm. 2.4] and it does not seem feasible to the author to make use of the remaining projections by adapting the proof. We are unaware of any way to remedy this problem and therefore restrict ourselves to analytic test functions as it is usual for expansions going beyond the subleading term.

For simplicity we further restrict ourselves to entire test functions $h : \mathbb{C} \to \mathbb{C}$ which satisfy $h(0) = 0$, i.e. there exist $\omega_m \in \mathbb{C}$, $m \in \mathbb{N}$, such that

$$h(z) = \sum_{m\in\mathbb{N}} \omega_m z^m, \tag{6.9}$$

for all $z \in \mathbb{C}$. The assumption that the functions are analytic on the whole complex plane is made to ease up the notation in some of the results. In fact one could compute a finite radius $R > 0$ such that analyticity in the disc $B_R(0)$ of radius R centred about the origin would suffice.

For entire test functions h, we obtain a d-term asymptotic expansion and show that the remaining term is of logarithmic order in the scaling parameter L.

Theorem 6.1. *Let $h : \mathbb{C} \to \mathbb{C}$ be an entire function satisfying $h(0) = 0$. Let $b \in [0,\infty[$, then the following asymptotic formula holds*

$$\mathrm{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[h\big(\mathbf{1}_{\Lambda_L}\,\mathrm{Op}(\psi^{(b)}\mathcal{D})\mathbf{1}_{\Lambda_L}\big)\big] = \sum_{m=0}^{d-1}(2L)^{d-m}A_{m,h,b} + O(\log L), \tag{6.10}$$

as $L \to \infty$. The coefficients $A_{m,h,b}$ are defined in (6.2). *The implied constant in the error term of order* $\log L$ *is independent of the ultraviolet cut-off parameter b.*

Remark 6.2. (a) The coefficients $A_{m,h,b}$, $m \in \{0, \dots, d-1\}$, of the d leading terms of the asymptotic expansion correspond to the geometric structure of the cube, where the operators $X_{m,k,b}$, cf. (6.2), are localisations to an approximate $(d-m+k)$-face of the cube Λ. The constant $c_{k,m}$ counts the number $2^m \frac{d!}{m!(d-m)!}$ of $(d-m)$-faces and multiplies it with the number $\frac{m!}{k!(m-k)!}$ of $(d-m+k)$-faces containing a given $(d-m)$-face. While the expression is quite abstract, we do not try to obtain more explicit expressions for the coefficients due to the following two reasons.

(b) Due to the matrix nature of the symbol, it is in general not possible to find an explicit integral representation even for the coefficient of the area term, i.e. $A_{1,h,b}$ in our case. This has been observed multiple times for smooth domains Λ and general symbols [Wid80, Wid85], as well as in the special case of the free Dirac operator in dimension three [FLS24].

(c) The coefficients $A_{m,h,b}$, $m \in \{0, \dots, d-1\}$, of the d leading terms of the asymptotic expansion, all depend on the chosen ultraviolet cut-off parameter b. In fact, in the case $m \in \{1, \dots, d-1\}$ one would expect the coefficients to be of order b^{d-m} in the cut-off parameter by a scaling argument, see also the main result of [FLS24].

Studying the term of logarithmic order requires several additional steps. As we are not able to fully extend the one-dimensional local asymptotic formula given in [Wid82] to our higher dimensional case, we are required to further restrict our choice of test functions in the last part of the proof contained in Section 6.6. The reason for this restriction is explained in more detail at the end of the next section and at the beginning of Section 6.6. For polynomial test functions h of degree less or equal than three, we are also able to compute the asymptotic coefficient of the subsequent logarithmic term and obtain the following $(d+1)$-term asymptotic expansion.

Theorem 6.3. *Let h be a polynomial of degree less or equal than three satisfying $h(0) = 0$. Let $b \in [0, \infty[$, then the following asymptotic formula holds*

$$\begin{aligned} \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \left[h\big(\mathbf{1}_{\Lambda_L} \operatorname{Op}(\psi^{(b)}\mathcal{D})\mathbf{1}_{\Lambda_L}\big)\right] = \sum_{m=0}^{d-1} (2L)^{d-m} A_{m,h,b} \\ + 2^d \log L \int_{S_+^{d-1}} \operatorname{tr}_{\mathbb{C}^n}[K_h(y,y)]\,\mathrm{d}y + O(1), \end{aligned} \tag{6.11}$$

as $L \to \infty$. Here, $S_+^{d-1} := \{y \in]0,\infty[^d : |y| = 1\} \subset S^{d-1}$ is the part of the unit sphere S^{d-1} which lies in the positive d-dimensional quadrant, and $K_h(y,y)$, $y \in S_+^{d-1}$ are the well-defined point-wise values of the continuous integral kernel K_h of the operator $\operatorname{Op}(\mathcal{D})_h$, which is given by

$$\operatorname{Op}(\mathcal{D})_h := \sum_{k=0}^{d} (-1)^k \sum_{\mathcal{M}\subseteq\{1,\dots,d\} \,:\, |\mathcal{M}|=k} h(\mathbf{1}_{H_\mathcal{M}} \operatorname{Op}(\mathcal{D})\mathbf{1}_{H_\mathcal{M}}), \tag{6.12}$$

with $H_\mathcal{M} := \{x \in \mathbb{R}^d : \forall j \in \{1,\dots,d\} \setminus \mathcal{M} : x_j \geqslant 0\}$.

We conclude this section by remarking upon some properties of the obtained asymptotic expansion.

Remark 6.4. (a) In contrast to the coefficients of the higher-order terms, the coefficient of the logarithmic term is independent of the cut-off parameter b. Therefore, we would indeed be interested to obtain a more explicit expression for it and maybe even relate it to the coefficients $\mathfrak{A}$ respectively $\mathfrak{U}$ which occur in the enhanced area laws obtained in Chapter 4. The reason why we are not able to do so, is again the lack of a full generalisation of the procedure in Section 6.6. The following two remarks point out similarities between these coefficients.

(b) For polynomials of degree one, the coefficient of the logarithmic term vanishes. This property is shared by the coefficient W in Theorem 5.1.

(c) For the second monomial g_2 and third monomial g_3, we have $\int_{S_+^{d-1}} \mathrm{tr}_{\mathbb{C}^n}[K_{g_3}(y,y)]\,\mathrm{d}y = \frac{3}{2}\int_{S_+^{d-1}} \mathrm{tr}_{\mathbb{C}^n}[K_{g_2}(y,y)]\,\mathrm{d}y$. This is the same ratio as for the coefficient W in Theorem 5.1, i.e. in Theorem 5.1 we have $W(g_3,\Lambda,E_F,m) = \frac{3}{2}W(g_2,\Lambda,E_F,m)$, independently of Λ, E_F and m. This is a consequence of the structure of the Dirac matrices, i.e. their vanishing trace and the anti-commutation relations (2.36), cf. Section 6.6.3. In fact, these properties allow even more insights on the coefficient for higher monomials: Under the assumption that Theorem 6.3 holds for all monomials of even degree g_{2k}, $k \in \{1,\dots,p\}$ for $p \in \mathbb{N}$, one can then deduce the theorem for the monomial g_{2p+1}. If the coefficient of the logarithmic term in (6.11) also obeys the desired ratio for the monomials g_{2k} and g_{2k-1}, $k \in \{2,\dots,p\}$, we would then obtain $\int_{S_+^{d-1}} \mathrm{tr}_{\mathbb{C}^n}[K_{g_{2p+1}}(y,y)]\,\mathrm{d}y = \big(1+(2p\sum_{k=1}^{2p-1}1/k)^{-1}\big)\int_{S_+^{d-1}} \mathrm{tr}_{\mathbb{C}^n}[K_{g_{2p}}(y,y)]\,\mathrm{d}y$. This is again the same ratio as for the coefficient W in Theorem 5.1. This fact could potentially be exploited in order to reduce the question of an explicit expression of the coefficient for the logarithmic term in (6.11) to just calculating it for the monomial of degree two. However, it is, at the moment, unclear to the author how to derive Theorem 6.3 for monomials of degree $2k$, $k \in \mathbb{N}\setminus\{1\}$, and we therefore do not pursue this route further in this chapter.

(d) Theorems 6.1 and 6.3 can be generalised to symbols B which feature not only a single point-discontinuity given by $\mathcal{D}$ but a finite number of such discontinuities in the compact support of the symbol B. The coefficient of the logarithmic term is then the sum of the coefficients corresponding to the points of discontinuity weighted by the values of B at these points. A proof of this fact is quite straightforward, as it just requires an additional localisation in momentum space, akin to the one used in the Widom–Sobolev formula, cf. Section 4.2, during the commutation procedure in Section 6.5. Still, we opt not to make this extension precise in this chapter, in order to maintain as much readability as possible in the already long Section 6.5.

(e) In order to obtain the first d terms of the expansions (6.10) and (6.11), we only make use of the fact that the operator $\mathrm{Op}(\psi^{(b)}\mathcal{D})$ has off-diagonal integral kernel decay of order $|x-y|^{-d}$ to obtain the required bounds and that the operator is translation-invariant with continuous integral kernel in order to evaluate the coefficients, cf. Theorem 6.8. No other, more specific, properties of the Dirac operator are required.

(f) The exact decay of order $|x-y|^{-d}$ required in Theorem 6.8 is crucial, in the sense that a higher order decay of order $|x-y|^{-\alpha}$ with $\alpha > d$ would already yield a full $(d+1)$-term asymptotic expansion, with the $(d+1)$st term being of constant order.

6.2. Properties of the integral kernel and strategy of the proof

In order to prove the desired asymptotic expansion, we combine methods from the analysis of both continuous and discontinuous symbols. In Section 6.3 we derive the first d terms of the expansion in a similar way as for continuous symbols. To do so, we require estimates for the off-diagonal decay of the integral kernel K of the operator $\mathrm{Op}(\psi\mathcal{D})$ which we obtain now. As multidimensional analogues of the Hilbert transform, the functions $\xi \mapsto -\mathrm{i}\frac{\xi_k}{|\xi|}$ are the Fourier multipliers corresponding to the kth d-dimensional Riesz transform, see [Ste70, p. 57] respectively [SW71, p. 223f.]. Hence, the kernel of the translation-invariant operator $\mathrm{Op}(\psi\mathcal{D})$ is given by

$$K(x) = \frac{\mathbb{1}_n}{2}\check{\psi}(x) + \frac{c_d}{2\mathrm{i}}\sum_{k=1}^{d}\alpha_k \lim_{\varepsilon\to 0}\int_{\mathbb{R}^d\setminus B_\varepsilon(x)} \frac{(x_k-t_k)\check{\psi}(t)}{|x-t|^{d+1}}\,\mathrm{d}t, \tag{6.13}$$

where $\check{\psi}$ denotes the inverse Fourier transform of the Schwartz function ψ and the constant c_d is given by $c_d := \frac{\Gamma[(d+1)/2]}{\pi^{(d+1)/2}}$. We want to study the decay of the (matrix) Hilbert-Schmidt norm of this kernel. To do so, let $R > 0$ and $|x| > 2R$, then, for every $k \in \{1, \dots, d\}$, integrating by parts yields the bound

$$\begin{aligned}
&\lim_{\varepsilon\to 0} \int_{\mathbb{R}^d \setminus B_\varepsilon(x)} \frac{(x_k - t_k)\check{\psi}(t)}{|x-t|^{d+1}} \, \mathrm{d}t \\
&= \int_{\mathbb{R}^d \setminus B_R(x)} \frac{(x_k - t_k)\check{\psi}(t)}{|x-t|^{d+1}} \, \mathrm{d}t + \lim_{\varepsilon\to 0} \int_{B_R(x) \setminus B_\varepsilon(x)} \frac{(x_k - t_k)\check{\psi}(t)}{|x-t|^{d+1}} \, \mathrm{d}t \\
&\leqslant \frac{C_1}{R^d} + \lim_{\varepsilon\to 0} \left[\int_{\partial(B_R(x)\setminus B_\varepsilon(x))} \frac{\check{\psi}(t)}{|x-t|^{d-1}} e_k \cdot \nu(t) \, \mathrm{d}S(t) - \int_{B_R(x)\setminus B_\varepsilon(x)} \frac{1}{|x-t|^{d-1}} \partial_k \check{\psi}(t) \, \mathrm{d}t \right] \\
&\leqslant \frac{C_1}{R^d} + C_2 \sup_{|t|\geqslant R} \left(|\check{\psi}(t)| + R \left| \partial_k \check{\psi}(t) \right| \right) \leqslant \frac{C_3}{R^d},
\end{aligned} \tag{6.14}$$

with constants $C_1, C_2, C_3 > 0$ independent of R, where we used that $\check{\psi}$ is a Schwartz function. Here, ∂ denotes the boundary of a set in $\mathbb{R}^d$, $\nu = \nu_{\partial(B_R(x)\setminus B_\varepsilon(x))}$ denotes the vector field of exterior unit normals in $\mathbb{R}^d$ to the boundary of $B_R(x) \setminus B_\varepsilon(x)$, and we write $\mathrm{d}S$ for integration with respect to the $(d-1)$-dimensional surface measure induced by Lebesgue measure in $\mathbb{R}^d$. Combining the estimates for every $k \in \{1, \dots, d\}$, we find a constant $C_4 > 0$, independent of x, such that the (matrix) Hilbert-Schmidt norm $\|K(x)\|_2$ is bounded from above by $\frac{C_4}{|x|^d}$. Being the inverse Fourier transform of the integrable function $\psi\mathcal{D}$, the kernel K is continuous. Interpreting K as a function $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}^{n\times n}$, the matrix Hilbert-Schmidt norm of its values is then bounded from above by

$$\|K(x,y)\|_2 \leqslant C_K \frac{1}{(1+|x-y|^2)^{\frac{d}{2}}}, \quad x, y \in \mathbb{R}^d, \tag{6.15}$$

for a constant $C_K > 0$. The continuity of the integral kernel of $\mathrm{Op}(\psi\mathcal{D})$, together with the just obtained decay estimate, ensures that the integral kernel of the operator $h\big(\mathbf{1}_M \mathrm{Op}(\psi\mathcal{D})\mathbf{1}_M\big)$ is also continuous on $M \times M$ for any open set $M \subseteq \mathbb{R}^d$ and entire test function h with $h(0) = 0$. We give a proof of this fact in Section 6.3.

We now remark upon the following symmetry properties of the operator $\mathrm{Op}(\psi\mathcal{D})$ which will be useful in the following sections. They rely on the fact that ψ is spherically symmetric.

Remark 6.5. (a) Symmetry of spatial directions: Given a permutation $\pi \in \mathcal{S}_d$, in the symmetric group of the set $\{1, \dots, d\}$, and the corresponding unitary operator U_π on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$ with action $(U_\pi u)(x) := u(\pi(x)) := u(x_{\pi(1)}, \dots, x_{\pi(d)})$, we have that

$$U_\pi \, \mathrm{Op}(\psi\mathcal{D}) U_\pi^{-1} = \mathrm{Op}(\psi\mathcal{D}_\pi), \tag{6.16}$$

where the symbol $\mathcal{D}_\pi = \frac{1}{2}\Big(\mathbb{1}_n - \sum_{k=1}^d \alpha_{\pi(k)} \frac{\xi_k}{|\xi|}\Big)$ agrees with the symbol $\mathcal{D}$ up to a relabelled choice of Dirac matrices. Therefore, for a measurable set $\Omega \subset \mathbb{R}^d$ and the corresponding set $\Omega_\pi := \{x \in \mathbb{R}^d : \ \pi(x) \in \Omega\}$, we have

$$\mathrm{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \big[\mathbf{1}_\Omega \, \mathrm{Op}(\psi\mathcal{D}) \mathbf{1}_\Omega\big] = \mathrm{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \big[\mathbf{1}_{\Omega_\pi} \, \mathrm{Op}(\psi\mathcal{D}) \mathbf{1}_{\Omega_\pi}\big]. \tag{6.17}$$

(b) Symmetry under reflections: Given $\sigma \in \{0,1\}^d$ and the corresponding unitary operator U_σ on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$ with action $(U_\sigma u)(x) := u(\sigma(x)) := u((-1)^{\sigma_1} x_1, \dots, (-1)^{\sigma_d} x_d)$, we have that

$$U_\sigma \, \mathrm{Op}(\psi\mathcal{D}) U_\sigma^{-1} = \mathrm{Op}(\psi\mathcal{D}_\sigma), \tag{6.18}$$

where the symbol $\mathcal{D}_\sigma = \frac{1}{2}\Big(\mathbb{1}_n - \sum_{k=1}^d (-1)^{\sigma_k}\alpha_k \frac{\xi_k}{|\xi|}\Big)$ agrees with the symbol $\mathcal{D}$ up to the signs of the chosen Dirac matrices. Therefore, for a measurable set $\Omega \subset \mathbb{R}^d$ and the corresponding set $\Omega_\sigma := \{x \in \mathbb{R}^d : \sigma(x) \in \Omega\}$, we have

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\mathbf{1}_\Omega \operatorname{Op}(\psi\mathcal{D})\mathbf{1}_\Omega\big] = \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\mathbf{1}_{\Omega_\sigma} \operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{\Omega_\sigma}\big]. \tag{6.19}$$

These properties can also be checked with the corresponding properties of the integral kernel, see [Ste70, p. 57]. They agree with the symmetry properties $(\mathcal{A}_2)$ and $(\mathcal{A}_3)$ in [Die18].

The analysis in Section 6.3 consists of an algebraic decomposition of the cube, which largely agrees with the decomposition in [Die18] and uses some methods from [Pfi19], as well as trace norm estimates for certain operators arising in this decomposition. The substantially worse decay of the kernel in our case, forces us to obtain these estimates in the following different way. For simplicity let us assume that we are in dimension $d = 2$, as the decomposition is relatively simple in this case. In higher dimensions a more careful analysis, as carried out in Section 6.3, is required. We subdivide the square $\Lambda_L = [0, 2L]^2$ into four smaller squares, each corresponding to one of the four vertices of Λ_L, and rewrite the studied operator as

$$\big(\mathbf{1}_{[0,L]^2} + \mathbf{1}_{[0,L]\times[L,2L]} + \mathbf{1}_{[L,2L]\times[0,L]} + \mathbf{1}_{[L,2L]^2}\big)h\big(\mathbf{1}_{\Lambda_L}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{\Lambda_L}\big), \tag{6.20}$$

where we used that $h(0) = 0$. Due to the symmetry of the problem, it suffices to study the contribution with the projection onto $[0, L]^2$ which stems from the vertex at the origin. Defining the half-spaces $H_1 := \mathbb{R}_+ \times \mathbb{R}$ and $H_2 := \mathbb{R} \times \mathbb{R}_+$, we rewrite this contribution in (6.20) as

$$\begin{aligned}
&\mathbf{1}_{[0,L]^2} h\big(\operatorname{Op}(\psi\mathcal{D})\big)\\
&+ \mathbf{1}_{[0,L]^2}\big[h\big(\mathbf{1}_{H_1}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_1}\big) - h\big(\operatorname{Op}(\psi\mathcal{D})\big)\big]\\
&+ \mathbf{1}_{[0,L]^2}\big[h\big(\mathbf{1}_{H_2}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_2}\big) - h\big(\operatorname{Op}(\psi\mathcal{D})\big)\big]\\
&+ \mathbf{1}_{[0,L]^2}\big[h\big(\mathbf{1}_{\Lambda_L}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{\Lambda_L}\big) - h\big(\mathbf{1}_{H_1}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_1}\big) - h\big(\mathbf{1}_{H_2}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_2}\big) + h\big(\operatorname{Op}(\psi\mathcal{D})\big)\big].
\end{aligned} \tag{6.21}$$

The operator in the first line of (6.21) will give rise to the volume term, the operators in the second and third line will give rise to the surface area terms and we will later see that the operator in the last line is of logarithmic order. Continuing our example, we now explain how one obtains the area term corresponding to the second term in (6.21). The idea is to replace the projection onto the square $[0, L]^2$ by a projection onto the semi-finite rectangle $\mathbb{R}_+ \times [0, L]$ and verify that this only incurs an error term of constant order. We begin by studying monomial test functions $h = g_p$, $p \in \mathbb{N}$. We note that

$$\big(\mathbf{1}_{H_1}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_1}\big)^p - \big(\operatorname{Op}(\psi\mathcal{D})\big)^p \tag{6.22}$$

can be written as a sum of operators, each containing at least one projection onto $(H_1)^c$, the complement of the half-space H_1. Therefore, the trace norm

$$\big\|\big(\mathbf{1}_{\mathbb{R}_+\times[0,L]} - \mathbf{1}_{[0,L]^2}\big)\big[\big(\mathbf{1}_{H_1}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_1}\big)^p - \big(\operatorname{Op}(\psi\mathcal{D})\big)^p\big]\big(\mathbf{1}_{\mathbb{R}_+\times[0,L]} - \mathbf{1}_{[0,L]^2}\big)\big\|_1 \tag{6.23}$$

can be estimated by a sum of products of Hilbert-Schmidt norms of the form

$$\big\|\big(\mathbf{1}_{\mathbb{R}_+\times[0,L]} - \mathbf{1}_{[0,L]^2}\big)\big(\mathbf{1}_{H_1}\operatorname{Op}(\psi\mathcal{D})\big)^k\mathbf{1}_{(H_1)^c}\big\|_2, \tag{6.24}$$

for $k \in \{1, \cdots, p-1\}$. We first consider the case $k = 1$. Noting that for any $x \in \mathbb{R}_+ \times [0, L] \setminus [0, L]^2 = [L, \infty[\times[0, L]$ the distance to $(H_1)^c$ is given by its first coordinate, i.e. $\operatorname{dist}(x, (H_1)^c) = x_1$, we see that the Hilbert-Schmidt norm (6.24) is of constant order in L as a direct consequence of the following

Lemma 6.6. *Let X be an integral operator, whose integral kernel satisfies inequality* (6.15). *Let $M, N \subset \mathbb{R}^d$ be measurable and such that there exists a measurable function $\varphi : \mathbb{R}^d \longrightarrow [0, \infty[$ with* $\operatorname{dist}(x, N) \geqslant \varphi(x)$ *for every $x \in M$, as well as a constant C_φ such that*

$$\int_M \frac{1}{(1+\varphi(x)^2)^{\frac{d}{2}}}\,\mathrm{d}x < C_\varphi. \tag{6.25}$$

Then the operator $\mathbf{1}_M X \mathbf{1}_N$ is Hilbert-Schmidt class with its Hilbert-Schmidt norm on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$ satisfying the bound

$$\|\mathbf{1}_M X \mathbf{1}_N\|_2^2 < C_\varphi C_d C_K^2, \tag{6.26}$$

where the constant C_K is the constant in the bound (6.15) *and the constant C_d only depends on the dimension d. Here,* dist *denotes the Euclidian distance in $\mathbb{R}^d$.*

Proof. It suffices to show that

$$\int_M \int_N \|K(x,y)\|_2^2 \,\mathrm{d}y\,\mathrm{d}x < C_\varphi C_d C_K^2. \tag{6.27}$$

We fix $x \in M$ and estimate the integral over the set N in the following way

$$\begin{aligned}\int_N \|K(x,y)\|_2^2\,\mathrm{d}y &\leqslant \int_N C_K^2 \frac{1}{(1+|x-y|^2)^d}\,\mathrm{d}y \leqslant C_K^2 \int_{\mathbb{R}^d \setminus B_{\varphi(x)}(x)} \frac{1}{(1+|x-y|^2)^d}\,\mathrm{d}y \\ &= C_K^2 \int_{\mathbb{R}^d \setminus B_{\varphi(x)}(0)} \frac{1}{(1+|y|^2)^d}\,\mathrm{d}y = C_K^2 |S^{d-1}| \int_{\varphi(x)}^\infty \frac{r^{d-1}}{(1+r^2)^d}\,\mathrm{d}r \\ &\leqslant C_K^2 |S^{d-1}| \int_{\varphi(x)}^\infty \frac{r}{(1+r^2)^{\frac{d}{2}+1}}\,\mathrm{d}r = \frac{C_K^2 |S^{d-1}|}{d} \frac{1}{(1+\varphi(x)^2)^{\frac{d}{2}}}.\end{aligned} \tag{6.28}$$

Here, $|S^{d-1}|$ denotes the $(d-1)$-dimensional surface area of the unit sphere S^{d-1} induced by Lebesgue measure. It follows that

$$\int_M \int_N \|K(x,y)\|_2^2\,\mathrm{d}y\,\mathrm{d}x \leqslant \frac{C_K^2 |S^{d-1}|}{d} \int_M \frac{1}{(1+\varphi(x)^2)^{\frac{d}{2}}}\,\mathrm{d}x < C_\varphi C_d C_K^2, \tag{6.29}$$

with $C_d := \frac{|S^{d-1}|}{d}$. □

For $k \geqslant 2$, estimating (6.24) is not as straightforward. But we still require Lemma 6.6 to do so. In order to still utilise the decay of the integral kernel, as well as the distance of the sets $[L, \infty[\times[0, L]$ and $(H_1)^c$, we use a quite technical procedure of constructing neighbourhoods of $[L, \infty[\times[0, L]$ whose boundaries locally are graphs of suitably chosen power functions $f(x) = x^q$ with $0 < q < 1$. We will now illustrate this procedure in the case $k = 2$. As neither the sets $[L, \infty[\times[0, L]$ and H_1 nor the sets H_1 and $(H_1)^c$ fulfil the requirements in order for Lemma 6.6 to yield an error term of constant order, we split the half-space H_1 into two parts. To do so, we introduce the function $\phi_L : \mathbb{R}_+ \longrightarrow \mathbb{R}_+$ given by

$$\phi_L(x) := \tfrac{1}{2} L^{\frac{1}{4}} x^{\frac{3}{4}} \tag{6.30}$$

and the set

$$H_{1,L,\phi} := \{x \in \mathbb{R}^d : \ x_2 \leqslant L + \phi_L(x_1) \text{ and } x_1 \geqslant \tfrac{L}{2}\}. \tag{6.31}$$

Checking the requirements of Lemma 6.6, we see that both the Hilbert-Schmidt norms

$$\big\|\big(\mathbf{1}_{\mathbb{R}_+\times[0,L]} - \mathbf{1}_{[0,L]^2}\big) \operatorname{Op}(\psi\mathcal{D})\big(\mathbf{1}_{H_1} - \mathbf{1}_{H_{1,L,\phi}}\big)\big\|_2 \quad \text{and} \quad \big\|\mathbf{1}_{H_{1,L,\phi}} \operatorname{Op}(\psi\mathcal{D}) \mathbf{1}_{(H_1)^c}\big\|_2, \tag{6.32}$$

are of constant order in L. This yields a bound of constant order for (6.24) in the case $k = 2$. For $k \geqslant 3$, we need to iterate this procedure, constructing in total $k-1$ functions and corresponding sets. How this procedure works in general, is best illustrated in the proof of Lemma 6.11. It also appears several times in the proofs in Section 6.5. Extending the estimate from monomials to entire functions, we obtain the operator

$$\mathbf{1}_{\mathbb{R}_+\times[0,L]}\big[h\big(\mathbf{1}_{H_1}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_1}\big)-h\big(\operatorname{Op}(\psi\mathcal{D})\big)\big]\mathbf{1}_{\mathbb{R}_+\times[0,L]}, \tag{6.33}$$

up to an error term of constant order. It remains to see that this operator is trace class and that it yields a term of order L in the asymptotic expansion. The fact that the operator (6.33) is trace class follows in similar fashion to the estimate of (6.23). Noting that the operator $h\big(\mathbf{1}_{H_1}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_1}\big)-h\big(\operatorname{Op}(\psi\mathcal{D})\big)$ is translation-invariant with respect to the coordinate x_2 and that it has continuous kernel, we see that

$$\begin{aligned}
&\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{\mathbb{R}_+\times[0,L]}\big[h\big(\mathbf{1}_{H_1}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_1}\big)-h\big(\operatorname{Op}(\psi\mathcal{D})\big)\big]\mathbf{1}_{\mathbb{R}_+\times[0,L]}\Big]\\
&\quad= L\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{\mathbb{R}_+\times[0,1]}\big[h\big(\mathbf{1}_{H_1}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_1}\big)-h\big(\operatorname{Op}(\psi\mathcal{D})\big)\big]\mathbf{1}_{\mathbb{R}_+\times[0,1]}\Big]\\
&\quad= L\lim_{L\to\infty}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{[0,L]\times[0,1]}\big[h\big(\mathbf{1}_{H_1}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_1}\big)-h\big(\operatorname{Op}(\psi\mathcal{D})\big)\big]\Big],
\end{aligned}\tag{6.34}$$

which is one of the contributions to the coefficient $A_{1,h,b}$ defined in (6.2).

After determining the first d terms of the expansion, we consider the remaining operator. Continuing our example in dimension $d = 2$, this is the operator

$$\mathbf{1}_{[0,L]^2}\big[h\big(\mathbf{1}_{\Lambda_L}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{\Lambda_L}\big)-h\big(\mathbf{1}_{H_1}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_1}\big)-h\big(\mathbf{1}_{H_2}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_2}\big)+h\big(\operatorname{Op}(\psi\mathcal{D})\big)\big] \tag{6.35}$$

from the last line of (6.21). The first step is to localise the operator by replacing the projections onto Λ_L by projections onto the positive quadrant $\mathbb{R}_+^2 = H_1 \cap H_2$. We show in Section 6.3 that this only incurs error terms of constant order. The proof of this fact is significantly easier than obtaining the higher-order terms, but also rests on a Hilbert-Schmidt estimate as in Lemma 6.6. We now restrict our example even further by assuming that the test function is given by the monomial of degree 2, i.e. $h = g_2$, as it makes the exposition significantly easier. Then the localised version of the operator (6.35) reads

$$\mathbf{1}_{[0,L]^2}\Big[\big(\mathbf{1}_{\mathbb{R}_+^2}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{\mathbb{R}_+^2}\big)^2-\big(\mathbf{1}_{H_1}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_1}\big)^2-\big(\mathbf{1}_{H_2}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_2}\big)^2+\big(\operatorname{Op}(\psi\mathcal{D})\big)^2\Big]. \tag{6.36}$$

Using the cyclic property of the trace, we see that this operator has the same trace as the operator

$$\mathbf{1}_{[0,L]^2}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{]-\infty,0]^2}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{[0,L]^2}. \tag{6.37}$$

We begin Section 6.4 by proving some additional estimates for smooth symbols, which are consequences of the results in [Sob14]. In particular, we see that if we just have a smooth symbol ψ, the trace norm

$$\big\|\mathbf{1}_{[0,L]^2}\operatorname{Op}(\psi)\mathbf{1}_{]-\infty,0]^2}\big\|_1 \tag{6.38}$$

is bounded from above by a constant independently of L. In a similar way as in Lemma 3.9, we manage to extend this to a bound for the trace norm

$$\big\|\mathbf{1}_{[0,L]^2}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{]-\infty,0]^2}\big\|_1 \tag{6.39}$$

which is logarithmic in L and, for L sufficiently large, independent of the support of $\psi = \psi^{(b)}$ (and with it independent of the cut-off parameter b). This yields the desired logarithmic upper bound for the remaining operator in the case $h = g_2$. For entire test functions the process is more complicated and contained in the proof of Theorem 6.18.

In Section 6.5 we continue working with the remaining operator, in our example $d = 2$, $h = g_2$, given by

$$\mathbf{1}_{[0,L]^2}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{]-\infty,0]^2}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{[0,L]^2}. \tag{6.40}$$

From now on we treat this operator as in the case of a discontinuous symbol, see e.g. [Wid82, Sob13, Sob15]. The first step is to commute all occurrences of the smooth symbol ψ to one side of the operator, i.e. we want to obtain the operator

$$\mathrm{Op}(\psi^2)\mathbf{1}_{[0,L]^2}\,\mathrm{Op}(\mathcal{D})\mathbf{1}_{\,]-\infty,0]^2}\,\mathrm{Op}(\mathcal{D})\mathbf{1}_{[0,L]^2}. \tag{6.41}$$

While doing so, we are only allowed to incur error terms of constant order. This restriction makes the task quite tricky, as direct commutation of $\mathrm{Op}(\psi)$ with $\mathbf{1}_{[0,L]^2}$ would yield an error of order L, cf. Lemma 3.6. Therefore, we somehow need to make use of the structure of the operators (6.40) and (6.41), as well as the decay of the integral kernel of the operator $\mathrm{Op}(\mathcal{D})$. Our strategy is to again construct suitable neighbourhoods but now of the boundary of $[0,L]^2$. We divide $[0,L]^2$ into the two sets

$$M_{L,q} := \{x \in [0,L]^2 : \mathrm{dist}(x, \partial[0,L]^2) < |x|^q - 1\} \qquad \text{and} \qquad [0,L]^2 \setminus M_{L,q}, \tag{6.42}$$

for some $q \in\,]0,1[$. Now, commutation of $\mathrm{Op}(\psi)$ with $\mathbf{1}_{[0,L]^2} - \mathbf{1}_{M_{L,q}}$ only incurs an error term of constant order, so it suffices to consider the operator

$$\mathbf{1}_{M_{L,q}}\,\mathrm{Op}(\mathcal{D})\mathbf{1}_{\,]-\infty,0]^2}\,\mathrm{Op}(\mathcal{D})\mathbf{1}_{M_{L,q}}. \tag{6.43}$$

We estimate its trace norm by the square of the Hilbert-Schmidt norm

$$\left\|\mathbf{1}_{M_{L,q}}\,\mathrm{Op}(\mathcal{D})\mathbf{1}_{\,]-\infty,0]^2}\right\|_2. \tag{6.44}$$

To estimate this, we require an analogous result to Lemma 6.6 but for the operator $\mathrm{Op}(\mathcal{D})$ which no longer has an integrable symbol. The integral kernel of the operator $\mathrm{Op}(\mathcal{D})$ is singular at the origin and only exists as a tempered distribution. Nonetheless, away from the origin we can treat it as a function on $\mathbb{R}^d$ and it is clearly homogeneous of degree $-d$. Hence, we obtain the estimate

$$\|K(x)\|_2 \leqslant C_K \frac{1}{|x|^d}, \qquad |x| > c > 0 \tag{6.45}$$

and, in analogy to Lemma 6.6,

Lemma 6.7. *Let X be an integral operator, whose integral kernel satisfies inequality* (6.45). *Let $M, N \subset \mathbb{R}^d$ be measurable such that there exists a measurable function $\varphi : \mathbb{R}^d \to]c,\infty[$ with* $\mathrm{dist}(x,N) \geqslant \varphi(x)$ *for every $x \in M$ and a constant C_φ such that*

$$\int_M \frac{1}{\varphi(x)^d}\,\mathrm{d}x < C_\varphi. \tag{6.46}$$

Then the operator $\mathbf{1}_M X \mathbf{1}_N$ is Hilbert-Schmidt class with its Hilbert-Schmidt norm on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$ satisfying the bound

$$\|\mathbf{1}_M X \mathbf{1}_N\|_2^2 < C_\varphi C_d C_K^2, \tag{6.47}$$

where the constant C_K is the constant in the bound (6.45) *and the constant C_d only depends on the dimension d.*

Proof. The proof is analogous to the proof of Lemma 6.6. It suffices to show that

$$\int_M \int_N \|K(x,y)\|_2^2\,\mathrm{d}y\,\mathrm{d}x < C_\varphi C_d C_K^2. \tag{6.48}$$

We fix $x \in M$ and estimate the integral over the set N in the following way

$$\begin{aligned}\int_N \|K(x,y)\|_2^2 \,\mathrm{d}y &\leqslant \int_N C_K^2 \frac{1}{|x-y|^{2d}} \,\mathrm{d}y \leqslant C_K^2 \int_{\mathbb{R}^d \setminus B_{\varphi(x)}(x)} \frac{1}{|x-y|^{2d}} \,\mathrm{d}y \\ &= C_K^2 \int_{\mathbb{R}^d \setminus B_{\varphi(x)}(0)} \frac{1}{|y|^{2d}} \,\mathrm{d}y = C_K^2 |S^{d-1}| \int_{\varphi(x)}^{\infty} \frac{r^{d-1}}{r^{2d}} \,\mathrm{d}r \\ &= \frac{C_K^2 |S^{d-1}|}{d} \frac{1}{\varphi(x)^d}. \end{aligned} \tag{6.49}$$

It follows that

$$\int_M \int_N \|K(x,y)\|_2^2 \,\mathrm{d}y \,\mathrm{d}x \leqslant \frac{C_K^2 |S^{d-1}|}{d} \int_M \frac{1}{\varphi(x)^d} \,\mathrm{d}x < C_\varphi C_d C_K^2, \tag{6.50}$$

with $C_d := \frac{|S^{d-1}|}{d}$. □

With this Lemma at hand, we see that (6.44) is of constant order in L, as $q < 1$. Extending this to monomial test functions of higher degree $p \geqslant 3$ again requires the construction of additional appropriately chosen neighbourhoods – not only of $\partial[0,L]^2$ but also of the boundaries of the half-spaces H_1, H_2, as the structure of the operator is no longer as simple as in (6.40). Doing this rigorously and in sufficient detail leads to the long and technical treatment in Section 6.5.

After the commutation, we further follow the strategy for discontinuous symbols in Section 6.6 and try to establish a local asymptotic formula. The integral kernel of the remaining operator is a generalisation of the kernel in the one-dimensional case, cf. [Wid82, (12)], where the occurring Hilbert transform is replaced by its higher dimensional analogues, the Riesz transforms. Therefore, the idea is to extend the original one-dimensional proof in [Wid82] to higher dimensions. While doing so, we face the challenge that the one-dimensional proof relies on a connection between Hilbert and Mellin transform which allows one to find the spectral representation of the operator in question. At this point, we need to restrict our chosen test functions, as we are not able to find a higher-dimensional analogue to this connection, due to the substantially more complex structure of the higher-dimensional operator and the unclear connection between the higher-dimensional transforms. Still, we are able to prove the required properties of the kernel by hand, in the special case that the test function is given by the monomial of degree two. We then continue by proving a local asymptotic formula under several assumptions on the integral kernel. The proof of this local asymptotic formula is an extension of the one-dimensional proof in [Wid82] to higher dimensions. As in the one-dimensional case we use the homogeneity of the integral kernel of $\mathrm{Op}(\mathcal{D})$, now of degree $-d$ instead of -1, in order to reduce the problem through a scaling argument. But instead of reducing the positive half-axis $]0,\infty[$ to the single point $\{1\}$, we reduce the positive quadrant $]0,\infty[^d$ to the $(d-1)$-dimensional set $S_+^{d-1} := \{y \in]0,\infty[^d : |y| = 1\}$. The more complex nature of this reduced set leads to additional requirements on the integral kernel which can be avoided in the one-dimensional case. Lastly, we extend the result from the monomial of degree two to the monomial of degree three, by using the structure of the Dirac matrices.

6.3. Localisation and higher-order terms

We begin by studying the higher-order terms of the expansion. The required analysis relies entirely on the fact that the integral kernel of the operator in question satisfies the bound (6.15) and does not use any additional properties of the Dirac operator. Therefore, we study the trace

$$\mathrm{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \left[g\left(\mathbf{1}_{\Lambda_L} X \mathbf{1}_{\Lambda_L}\right) \right], \tag{6.51}$$

in the more general setting that X is a bounded translation-invariant integral operator on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$ with continuous integral kernel $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}^n$ satisfying the bound (6.15).

In this section we decompose the d-dimensional cube $\Lambda = [0, 2]^d$ in a similar way as in [Die18]. To do so, we first fix some notation. As usual, for $k \in \{-1, \dots, d\}$, we say that $F \subseteq \mathbb{R}^d$ is a k-face (of Λ) if $\dim(F) = k$ and there exists a half-space $H_F \subseteq \mathbb{R}^d$ with $\Lambda^\circ \cap \partial H_F = \varnothing$ such that $F = \Lambda \cap H_F$. Here, $^\circ$ denotes the interior of a set, $\dim(F)$ the dimension of the smallest affine subspace of $\mathbb{R}^d$ which contains F, $\varnothing$ the empty set and we define $\dim(\varnothing) := -1$. For each $k \in \{-1, \dots, d\}$, we denote by $\mathcal{F}^{(k)}$ the set of all k-faces of Λ. For a given j-face F, we define the sets $\mathcal{F}_F^{(k)} := \{G \in \mathcal{F}^{(k)} : F \subseteq G\}$ of all k-faces containing F for $k \in \{j, \dots, d\}$.

To the only d-face $F = \Lambda$ we associate the space $H_F = \mathbb{R}^d$. To each $(d-1)$-face $F \in \mathcal{F}^{(d-1)}$, we associate the unique half-space $H_F \subseteq \mathbb{R}^d$ such that $F \subset \partial H_F$ and $\Lambda \subset H_F$. For $k \in \{0, \dots, d-2\}$, we associate to a given k-face $F \in \mathcal{F}^{(k)}$ the space $H_F := \bigcap_{G \in \mathcal{F}_F^{(d-1)}} H_G$.

For a given k-Face F, $k \in \{1, \dots, d-1\}$, the smallest affine subspace W_F' of $\mathbb{R}^d$ with $F \subset W_F'$ is given by $W_F' = \bigcap_{G \in \mathcal{F}_F^{(d-1)}} \partial H_G$. We then find $u_F \in \mathbb{R}^d$ and a k-dimensional subspace W_F of $\mathbb{R}^d$ such that $W_F' = u_F + W_F$. Writing $\mathbb{R}^d \ni x = x_1 + x_2 \in (u_F + W_F) \oplus W_F^\intercal =: W_F' \oplus W_F^\intercal$, we define the semi-finite space $H_{F,\infty} := \{x_1 + x_2 \in H_F \subseteq W_F' \oplus W_F^\intercal : x_1 \in F\}$ as well as its finite scaled version $H_{F,L} := \{x_1 + x_2 \in H_F \subseteq W_F' \oplus W_F^\intercal : x_1 \in F,\ \|x_2\|_\infty \leqslant L\}$, where $\|\cdot\|_\infty$ denotes the maximum norm in $W_F^\intercal$.

We start by decomposing the scaled cube Λ_L into 2^d parts; each associated to one of the vertices (or 0-faces) of Λ. Let $V \in \mathcal{F}^{(0)}$ be any of these vertices. We begin by considering the finite scaled version of the space H_V associated to V, i.e. the cube $H_{V,L} = H_V \cap \big(V + [-L, L]^d\big)$ defined above. As $g(0) = 0$, we obtain

$$g\big(\mathbf{1}_{\Lambda_L} X \mathbf{1}_{\Lambda_L}\big) = \mathbf{1}_{\Lambda_L} g\big(\mathbf{1}_{\Lambda_L} X \mathbf{1}_{\Lambda_L}\big) = \sum_{V \in \mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}} g\big(\mathbf{1}_{\Lambda_L} X \mathbf{1}_{\Lambda_L}\big). \tag{6.52}$$

Let $m \in \{0, \dots, d\}$. For a given $(d-m)$-face F, we define the operator

$$X_{F,g} := \sum_{k=0}^{m} (-1)^k \sum_{G \in \mathcal{F}_F^{(k+(d-m))}} g(\mathbf{1}_{H_G} X \mathbf{1}_{H_G}) \tag{6.53}$$

and note that, for a given vertex V, we have

$$\sum_{m=0}^{d} \sum_{F \in \mathcal{F}_V^{(d-m)}} X_{F,g} = \sum_{m=0}^{d} \sum_{F \in \mathcal{F}_V^{(d-m)}} \sum_{k=0}^{m} (-1)^k \sum_{G \in \mathcal{F}_F^{(k+(d-m))}} g(\mathbf{1}_{H_G} X \mathbf{1}_{H_G}) = g(\mathbf{1}_{H_V} X \mathbf{1}_{H_V}), \tag{6.54}$$

as all other terms cancel out. Using this, we rewrite the right-hand side of (6.52) as

$$\sum_{V \in \mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}} \left[g\big(\mathbf{1}_{\Lambda_L} X \mathbf{1}_{\Lambda_L}\big) - g(\mathbf{1}_{H_V} X \mathbf{1}_{H_V}) + \sum_{m=0}^{d} \sum_{F \in \mathcal{F}_V^{(d-m)}} X_{F,g} \right]. \tag{6.55}$$

The first step will be to localise the operator up to a term of constant order, i.e. to show that for each vertex V, replacing $\mathbf{1}_{H_{V,L}} g\big(\mathbf{1}_{\Lambda_L} X \mathbf{1}_{\Lambda_L}\big)$ with $\mathbf{1}_{H_{V,L}} g(\mathbf{1}_{H_V} X \mathbf{1}_{H_V})$ in the trace of (6.55) only yields an error term of constant order in L. We will do this in Section 6.3.1. After the localisation we obtain

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \left[g\big(\mathbf{1}_{\Lambda_L} X \mathbf{1}_{\Lambda_L}\big) \right] = \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \left[\sum_{V \in \mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}} \left(X_{V,g} + \sum_{m=0}^{d-1} \sum_{F \in \mathcal{F}_V^{(d-m)}} X_{F,g} \right) \right], \tag{6.56}$$

up to an error term of constant order. As we will show in Section 6.4, the contributions to the higher-order terms stem exclusively from the sum

$$\sum_{V\in\mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}} \sum_{m=0}^{d-1} \sum_{F\in\mathcal{F}_V^{(d-m)}} X_{F,g}, \tag{6.57}$$

while the terms containing the operators $X_{V,g}$ are of logarithmic order in the scaling parameter L. The largest part of the present section is devoted to determining these higher-order terms, starting from the trace of (6.57). The results are summarised in the following

Theorem 6.8. *Let X be a bounded translation-invariant integral operator on $L^2(\mathbb{R}^d)\otimes\mathbb{C}^n$ with continuous integral kernel $K:\mathbb{R}^d\times\mathbb{R}^d\to\mathbb{C}^n$ satisfying the bound* (6.15)*. Let $g:\mathbb{C}\to\mathbb{C}$ be an entire function with $g(0)=0$. Further let $\Lambda=[0,2]^d\subset\mathbb{R}^d$. Then*

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}&\Big[g\big(\mathbf{1}_{\Lambda_L}X\mathbf{1}_{\Lambda_L}\big)-\sum_{V\in\mathcal{F}^{(0)}}\mathbf{1}_{H_{V,L}}X_{V,g}\Big]\\ &=\sum_{m=0}^{d-1}L^{d-m}\lim_{L\to\infty}\sum_{F\in\mathcal{F}^{(d-m)}}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\mathbf{1}_{H_{F,L}}X_{F,g}\big]+O(1),\end{aligned}\tag{6.58}$$

as $L\to\infty$. If the operator X additionally fulfils the symmetry properties in Remark 6.5*, this reduces to*

$$\begin{aligned}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}&\Big[g\big(\mathbf{1}_{\Lambda_L}X\mathbf{1}_{\Lambda_L}\big)-\sum_{k=0}^{d}c_{k,d}\mathbf{1}_{[0,L]^d}g\big(\mathbf{1}_{\mathbb{R}_+^{d-k}\times\mathbb{R}^k}X\mathbf{1}_{\mathbb{R}_+^{d-k}\times\mathbb{R}^k}\big)\Big]\\ =\sum_{m=0}^{d-1}&(2L)^{d-m}\lim_{L\to\infty}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\sum_{k=0}^{m}c_{k,m}\mathbf{1}_{[0,L]^m\times[0,1]^{d-m}}g\big(\mathbf{1}_{\mathbb{R}_+^{m-k}\times\mathbb{R}^{d-m+k}}X\mathbf{1}_{\mathbb{R}_+^{m-k}\times\mathbb{R}^{d-m+k}}\big)\Big]\\ &+O(1),\end{aligned}\tag{6.59}$$

as $L\to\infty$, with the constants $c_{k,m}:=\frac{(-1)^k2^md!}{k!(m-k)!(d-m)!}$ for $0\leqslant k\leqslant m\leqslant d$. The limits of the operators in the traces on the right-hand side of both (6.58) *and* (6.59) *are only trace class in the case $m=0$. Therefore, the limit can not be exchanged with the trace.*

The proof of this theorem is divided into several steps. As mentioned above, we begin by localising the remaining operator in Section 6.3.1. Then we establish several required estimates for the operator X in Section 6.3.2. This will be the most challenging part of the proof. Lastly, we finish the proof of Theorem 6.8 in Section 6.3.3.

Throughout the proof of Theorem 6.8 we will often choose a designated vertex V and face F in the following way: Up to suitable rotation and translation, we can assume that the cube is still given by $\Lambda=[0,2]^d$, the vertex is given by $V=V_0=\{0\}\in\mathbb{R}^d$ and the $(d-m)$-face is given by $F=\{0\}^m\times[0,2]^{d-m}$. This will considerably simplify the notation in the following analysis. The sets, already defined in this section, are then given by

$$H_V=\mathbb{R}_+^d,\quad H_{V,L}=[0,L]^d,\quad H_F=\mathbb{R}_+^m\times\mathbb{R}^{d-m},\qquad H_{F,L}=[0,L]^m\times[0,2]^{d-m}. \tag{6.60}$$

6.3.1. Localisation in position space. We now study the absolute value of the trace of the operator

$$\sum_{V\in\mathcal{F}^{(0)}}\mathbf{1}_{H_{V,L}}\big[g(\mathbf{1}_{H_V}X\mathbf{1}_{H_V})-g\big(\mathbf{1}_{\Lambda_L}X\mathbf{1}_{\Lambda_L}\big)\big] \tag{6.61}$$

and show that it is bounded by a constant independently of the scaling parameter L. By the triangle inequality, it suffices to show this for the designated vertex $V = V_0$ chosen above, i.e. for the operator

$$\mathbf{1}_{[0,L]^d}\Big(g\big(\mathbf{1}_{\mathbb{R}^d_+}\mathbf{1}_{\mathbb{R}^d_+}\big) - g\big(\mathbf{1}_{\Lambda_L}X\mathbf{1}_{\Lambda_L}\big)\Big). \tag{6.62}$$

The proof is given in the following two lemmas. The first one gives a Hilbert-Schmidt estimate, in a more general setting for monomial test function, and the second one applies this to the operator in question and yields an estimate for the absolute value of the trace of (6.62).

Lemma 6.9. *Let $L \geqslant 1$. Let $p \in \mathbb{N}$, $\Omega_1, \dots, \Omega_p \subseteq \mathbb{R}^d$ be measurable and $X_1, \dots, X_p$ be bounded translation-invariant integral operators on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$, each satisfying estimate* (6.45). *Further let $M, N \subset \mathbb{R}^d$ be measurable and such that there exist constants $\rho, R > 0$, independent of L, with $M \subset B_{L\rho}(0)$ and $\operatorname{dist}(M, N) > RL$. Then there exists a constant $C > 0$, independent of L and p, such that*

$$\Big\|\mathbf{1}_M\Big(\prod_{m=1}^{p}\mathbf{1}_{\Omega_m}X_m\Big)\mathbf{1}_N\Big\|_2 \leqslant Cp^{\frac{d+2}{2}}\Big(\max_{1\leqslant m\leqslant p}\|X_m\|\Big)^{p-1}. \tag{6.63}$$

Proof. We start with the case $p = 1$. The sets $M \cap \Omega_1$ and N satisfy the requirements of Lemma 6.7 with $\varphi(x) = RL$. As

$$\int_{M\cap\Omega_1}\frac{1}{\varphi(x)^d}\,\mathrm{d}x \leqslant \int_{B_{L\rho}(0)}\frac{1}{(RL)^d}\,\mathrm{d}x = |B_1(0)|\frac{\rho^d}{R^d}, \tag{6.64}$$

Lemma 6.7 yields a constant $C > 0$, independent of L, such that

$$\big\|\mathbf{1}_M\mathbf{1}_{\Omega_1}X_1\mathbf{1}_N\big\|_2 < C. \tag{6.65}$$

In order to prove the case $p \geqslant 2$, we construct $p-1$ sets "in between" the sets M and N. Namely, we define the sets $M_k := \{x \in \Omega_k : \operatorname{dist}(x, M) \leqslant \frac{(k-1)R}{p}L\}$, for $k \in \{1, \dots, p\}$. We note that $M_1 = M$. Clearly, we have $\operatorname{dist}\big(M_k, \Omega_{k+1} \setminus M_{k+1}\big) > \frac{R}{p}L$, for all $k \in \{1, \dots, p-1\}$. Defining $\varphi(x) := \frac{R}{p}L$, we calculate

$$\int_{M_k}\frac{1}{\varphi(x)^d}\,\mathrm{d}x \leqslant \int_{B_{L(\rho+R)}(0)}\frac{p^d}{(RL)^d} = p^d|B_1(0)|\frac{(\rho+R)^d}{R^d}, \tag{6.66}$$

for $k \in \{1, \dots, p-1\}$, and Lemma 6.7 yields a constant $C_k > 0$, independent of L and p, such that

$$\big\|\mathbf{1}_{M_k}X_k\mathbf{1}_{\Omega_{k+1}\setminus M_{k+1}}\big\|_2 \leqslant C_k\sqrt{p^d}. \tag{6.67}$$

As we also have $\operatorname{dist}\big(M_p, N\big) > \frac{R}{p}L$, Lemma 6.7 yields a constant $C_p > 0$, independent of L and p, with

$$\big\|\mathbf{1}_{M_p}X_p\mathbf{1}_N\big\|_2 \leqslant C_p\sqrt{p^d}, \tag{6.68}$$

in the same way. Repeated use of the triangle inequality, followed by Hölder's inequality and application of the bounds (6.67) and (6.68), yields

$$\begin{aligned}
&\Big\|\mathbf{1}_M\Big(\prod_{m=1}^{p}\mathbf{1}_{\Omega_m}X_m\Big)\mathbf{1}_N\Big\|_2\\
&\quad\leqslant\sum_{j=1}^{p-1}\Big\|\Big(\prod_{k=1}^{j}\mathbf{1}_{M_k}X_k\Big)\mathbf{1}_{\Omega_{j+1}\setminus M_{j+1}}X_{j+1}\Big(\prod_{k=j+2}^{p}\mathbf{1}_{\Omega_k}X_k\Big)\mathbf{1}_N\Big\|_2+\Big\|\Big(\prod_{k=1}^{p}\mathbf{1}_{M_k}X_k\Big)\mathbf{1}_N\Big\|_2\\
&\quad\leqslant\sum_{j=1}^{p-1}\big\|\mathbf{1}_{M_k}X_k\mathbf{1}_{\Omega_{k+1}\setminus M_{k+1}}\big\|_2\Big(\max_{1\leqslant m\leqslant p}\|X_m\|\Big)^{p-1}+\big\|\mathbf{1}_{M_p}X_p\mathbf{1}_N\big\|_2\Big(\max_{1\leqslant m\leqslant p}\|X_m\|\Big)^{p-1}\\
&\quad\leqslant Cp^{\frac{d+2}{2}}\Big(\max_{1\leqslant m\leqslant p}\|X_m\|\Big)^{p-1},
\end{aligned}\tag{6.69}$$

with a constant $C>0$, independent of L and p. This proves the lemma for $p\geqslant 2$. □

Lemma 6.10. *Let $L\geqslant 1$, $g:\mathbb{C}\to\mathbb{C}$ be an entire function with $g(0)=0$ and X be a bounded translation-invariant integral operator on $L^2(\mathbb{R}^d)\otimes\mathbb{C}^n$ whose integral kernel satisfies estimate* (6.45)*. Then there exists a constant $C>0$, independent of L, such that*

$$\Big|\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{[0,L]^d}\Big(g\big(\mathbf{1}_{\mathbb{R}^d_+}X\mathbf{1}_{\mathbb{R}^d_+}\big)-g\big(\mathbf{1}_{\Lambda_L}X\mathbf{1}_{\Lambda_L}\big)\Big)\Big]\Big|\leqslant C.\tag{6.70}$$

Proof. We start with a proof for monomial test functions g. Let $p\in\mathbb{N}$ and set $P_0:=\mathbf{1}_{\Lambda_L}$ as well as $P_1:=\mathbf{1}_{\mathbb{R}^d_+}$. Using the fact that $\mathbf{1}_{[0,L]^d}P_0=\mathbf{1}_{[0,L]^d}P_1=\mathbf{1}_{[0,L]^d}$ and the cyclic property of the trace, we rewrite the operator in (6.70) as

$$\mathbf{1}_{[0,L]^d}\big[(XP_0)^{p-1}-(XP_1)^{p-1}\big]X\mathbf{1}_{[0,L]^d}\tag{6.71}$$

and see that in the case $p=1$ there is nothing to show. If $p\geqslant 2$, we define $P_2=P_1-P_0=\mathbf{1}_{\mathbb{R}^d_+\setminus[0,2L]^d}$ and write

$$\begin{aligned}
&\mathbf{1}_{[0,L]^d}(XP_1)^{p-1}X\mathbf{1}_{[0,L]^d}\\
&\qquad=\mathbf{1}_{[0,L]^d}(XP_0+XP_2)^{p-1}X\mathbf{1}_{[0,L]^d}\\
&\qquad=\sum_{\pi=(\pi_1,\dots,\pi_{p-1})\in\{0,2\}^{p-1}}\mathbf{1}_{[0,L]^d}\Big(\prod_{j=1}^{p-1}XP_{\pi(j)}\Big)X\mathbf{1}_{[0,L]^d}.
\end{aligned}\tag{6.72}$$

With this at hand, we estimate the trace norm of (6.71) by

$$\sum_{\pi\in\{0,2\}^{p-1}:\ \pi\neq 0}\Big\|\mathbf{1}_{[0,L]^d}\Big(\prod_{j=1}^{p-1}XP_{\pi(j)}\Big)X\mathbf{1}_{[0,L]^d}\Big\|_1.\tag{6.73}$$

Each of these trace norms contains at least one factor P_2. Setting $p_{1,\pi}:=\min\{j\in\{1,\dots,p-1\}:\pi(j)=2\}$ and $p_{2,\pi}:=\max\{j\in\{1,\dots,p-1\}:\ \pi(j)=2\}$ for a given $\pi\in\{0,2\}^{p-1}$ with $\pi\neq 0$, we estimate (6.73) by

$$\|X\|^{p-1-p_{1,\pi}-p_{2,\pi}}\sum_{\pi\in\{0,2\}^{p-1}:\ \pi\neq 0}\Big\|\mathbf{1}_{[0,L]^d}(P_0X)^{p_{1,\pi}}P_2\Big\|_2\Big\|P_2(XP_0)^{p_{2,\pi}}\mathbf{1}_{[0,L]^d}\Big\|_2.\tag{6.74}$$

By Lemma 6.9, there exists a constant $C_1>0$, independent of L and p, such that (6.74) is bounded by

$$C_1\sum_{\pi\in\{0,2\}^{p-1}:\ \pi\neq 0}(p_{1,\pi})^{\frac{d+2}{2}}(p_{2,\pi})^{\frac{d+2}{2}}\|X\|^{p-1}\leqslant C_1(p-1)^{d+2}(2\|X\|)^{p-1}.\tag{6.75}$$

This concludes the proof of the Lemma for monomials. It remains to extend it to entire functions g. With estimate (6.75) we write

$$\begin{aligned}
&\Big|\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{[0,L]^d}\Big(g\big(\mathbf{1}_{\mathbb{R}^d_+}X\mathbf{1}_{\mathbb{R}^d_+}\big)-g\big(\mathbf{1}_{\Lambda_L}X\mathbf{1}_{\Lambda_L}\big)\Big)\Big]\Big|\\
&\qquad=\Big|\sum_{p=1}^{\infty}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\omega_p\mathbf{1}_{[0,L]^d}\Big(\big(\mathbf{1}_{\mathbb{R}^d_+}X\mathbf{1}_{\mathbb{R}^d_+}\big)^p-\big(\mathbf{1}_{\Lambda_L}X\mathbf{1}_{\Lambda_L}\big)^p\Big)\Big]\Big|\\
&\qquad\leqslant C_2\sum_{p=1}^{\infty}|\omega_p|(p-1)^{d+2}(2\|X\|)^{p-1}\leqslant C, \qquad (6.76)
\end{aligned}$$

with constants $C, C_2>0$ independent of L. This concludes the proof of the Lemma. □

6.3.2. Hilbert-Schmidt and trace norm estimates. We continue with the proof of Theorem 6.8. We start by discussing the further strategy of the proof and by introducing some additional notation, before we prove the required bounds.

For each k-face F, we divide the sets $H_{F,\infty}$ and $H_{F,L}$ into 2^k parts, each associated to one of the 2^k vertices $V\in F$, given by $H_{F,L,V} := \{x_1+x_2 \in H_F \subseteq W_F'\oplus W_F^{\top} : x_1\in F\cap(V+[-1,1]^d),\ \|x_2\|_\infty\leqslant L\}$ for $L\in[1,\infty]$. Clearly, we have $H_{F,L}=\sum_{\{V\in\mathcal{F}^{(0)}:V\in F\}}H_{F,L,V}$. With this, (6.56) and the localisation in Section 6.3.1, we see that the proof of (6.58) reduces to showing that

$$\begin{aligned}
&\sum_{m=0}^{d-1}\sum_{V\in\mathcal{F}^{(0)}}\sum_{F\in\mathcal{F}_V^{(d-m)}}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\mathbf{1}_{H_{V,L}}X_{F,g}\big]\\
&\qquad=\sum_{m=0}^{d-1}L^{d-m}\lim_{L\to\infty}\sum_{V\in\mathcal{F}^{(0)}}\sum_{F\in\mathcal{F}_V^{(d-m)}}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\mathbf{1}_{H_{F,L,V}}X_{F,g}\big]+O(1), \qquad (6.77)
\end{aligned}$$

as $L\to\infty$. Therefore, for a given vertex $V\in\mathcal{F}^{(0)}$ and a given $(d-m)$-face F we need to show that the limit $L^{d-m}\lim_{L\to\infty}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\mathbf{1}_{H_{F,L,V}}X_{F,g}\big]$ exists and agrees with the trace $\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\mathbf{1}_{H_{V,L}}X_{F,g}\big]$ up to an error term of constant order.

It will again be convenient to only deal with the case, where the vertex is given by $V=\{0\}\in\mathbb{R}^d$ and the $(d-m)$-face is given by $F=\{0\}^m\times[0,2]^{d-m}$. The other cases reduce to this case after suitable rotation and translation. We recall that in this case we have

$$H_V=\mathbb{R}^d_+,\quad H_{V,L}=[0,L]^d,\quad H_F=\mathbb{R}^m_+\times\mathbb{R}^{d-m},\quad H_{F,L,V}=[0,L]^m\times[0,1]^{d-m}. \qquad (6.78)$$

We further note that in this case we also have $H_{F,\infty,V}=\mathbb{R}^m_+\times[0,1]^{d-m}$ for the recently defined set $H_{F,\infty,V}$ and define a scaled version of this set by $H_{F,\infty,V,L}:=(H_{F,\infty,V})_L=\mathbb{R}^m_+\times[0,L]^{d-m}$.

For the remaining part of the present section, we only deal with the case $m\in\{1,\dots,d-1\}$ and exclude the easier case $m=0$. In order to understand the structure of the operator $X_{F,g}$, it will be convenient to relabel the occurring projections. There is a one to one correspondence between the faces $G\in\mathcal{F}_F^{(k)}$, with $k\geqslant d-m$, and the sets $\mathcal{M}_G\subseteq\{1,\dots,m\}$ with $|\mathcal{M}_G|=k-(d-m)$. For a given set $\mathcal{M}\subseteq\{1,\dots,m\}$, we write $H_{\mathcal{M}}:=H_{\mathcal{M}_G}:=\{x\in\mathbb{R}^d : \forall j\in\{1,\dots,m\}\setminus\mathcal{M}_G : x_j\geqslant 0\}=H_G$. We note that the set $H_{\mathcal{M}}$ implicitly depends on the face F. Still, it is convenient to not reflect this dependence in the notation. With this, the operator $X_{F,g}$ is given by

$$X_{F,g}=\sum_{k=0}^{m}(-1)^k\sum_{\mathcal{M}\subseteq\{1,\dots,m\}\,:\,|\mathcal{M}|=k}g(\mathbf{1}_{H_{\mathcal{M}}}X\mathbf{1}_{H_{\mathcal{M}}}). \qquad (6.79)$$

Before we state the desired estimates, we subdivide the sets $H_{V,L}$ and $H_{F,\infty,V,L}$ into m different parts. Let $k \in \{1,\ldots,m\}$, then we define the sets

$$H_{L,m,k} := \{x \in H_{V,L} = [0,L]^d : \forall j \in \{1,\ldots,m\} \setminus \{k\} : x_j \leqslant x_k\} \tag{6.80}$$

and

$$H_{\infty,L,m,k} := \{x \in H_{F,\infty,V,L} = \mathbb{R}_+^m \times [0,L]^{d-m} : \forall j \in \{1,\ldots,m\} \setminus \{k\} : x_j \leqslant x_k\}. \tag{6.81}$$

We note that we drop the dependence on the vertex V and the face F in these sets, as we will only use the notation for the designated vertex $V = \{0\}$ and $(d-m)$-face $F = \{0\}^m \times [0,2]^{d-m}$. Rearranging the terms of the operator $X_{F,g}$, we obtain

$$\mathbf{1}_{H_{V,L}} X_{F,g} = \sum_{k=1}^m \mathbf{1}_{H_{L,m,k}} \sum_{\mathcal{M} \subseteq \{1,\ldots,m\}\setminus\{k\}} (-1)^{|\mathcal{M}|} \big[g\big(\mathbf{1}_{H_{\mathcal{M}}} X \mathbf{1}_{H_{\mathcal{M}}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\big] \tag{6.82}$$

as well as

$$\mathbf{1}_{H_{F,\infty,V,L}} X_{F,g} = \sum_{k=1}^m \mathbf{1}_{H_{\infty,L,m,k}} \sum_{\mathcal{M} \subseteq \{1,\ldots,m\}\setminus\{k\}} (-1)^{|\mathcal{M}|} \big[g\big(\mathbf{1}_{H_{\mathcal{M}}} X \mathbf{1}_{H_{\mathcal{M}}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\big]. \tag{6.83}$$

We now want to show that the operator

$$\mathbf{1}_{H_{\infty,L,m,k}} \big[g\big(\mathbf{1}_{H_{\mathcal{M}}} X \mathbf{1}_{H_{\mathcal{M}}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\big] \mathbf{1}_{H_{\infty,L,m,k}} \tag{6.84}$$

is trace class and analyse the operator difference

$$\big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big) \big[g\big(\mathbf{1}_{H_{\mathcal{M}}} X \mathbf{1}_{H_{\mathcal{M}}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\big] \big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big) \tag{6.85}$$

for given $k, m, \mathcal{M}$ and g. We do this in several lemmas in the present section.

We start with monomial test functions g and extend the result to analytic test functions in Lemma 6.13. As Lemma 6.12 shows, the expressions above can, for a given monomial g, be rewritten as a sum of terms which always contain at least one occurrence of the projection $\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} - \mathbf{1}_{H_{\mathcal{M}}}$. The following very technical Lemma 6.11 uses Lemma 6.6 to estimate the Hilbert-Schmidt norm of such terms. This constitutes the most challenging part of the proof of Theorem 6.8.

Lemma 6.11. *Let X be a bounded integral operator whose kernel satisfies the bound* (6.15). *Let $1 \leqslant k \leqslant m < d$ and $\mathcal{M} \subseteq \{1,\ldots,m\}$ such that $k \notin \mathcal{M}$. Let $L \geqslant 1$ and $p \in \mathbb{N}$. Then the operator*

$$\mathbf{1}_{H_{\infty,L,m,k}} (\mathbf{1}_{H_{\mathcal{M}}} X)^p (\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} - \mathbf{1}_{H_{\mathcal{M}}}) \tag{6.86}$$

is Hilbert-Schmidt class and there exists a constant $C > 0$, independent of L and p, such that

$$\|\mathbf{1}_{H_{\infty,L,m,k}} (\mathbf{1}_{H_{\mathcal{M}}} X)^p (\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} - \mathbf{1}_{H_{\mathcal{M}}})\|_2 \leqslant C \|X\|^{p-1} d^{\frac{p}{2}} p^{d+1} L^{\frac{d-m}{2}}. \tag{6.87}$$

Furthermore, there exists a constant $C' > 0$ which is independent of L and p such that

$$\|\big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big)(\mathbf{1}_{H_{\mathcal{M}}} X)^p (\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} - \mathbf{1}_{H_{\mathcal{M}}})\|_2 \leqslant C' \|X\|^{p-1} d^{\frac{p}{2}} p^{d+1}. \tag{6.88}$$

Proof. Let $L \geqslant 1$. We start by proving that the operator (6.86) is Hilbert-Schmidt. Due to the fact that $\mathbf{1}_{H_{\infty,L,m,k}} \mathbf{1}_{H_{\mathcal{M}}} = \mathbf{1}_{H_{\infty,L,m,k}}$, there are total of $p-1$ occurrences of the projection $\mathbf{1}_{H_{\mathcal{M}}}$ in (6.86). In particular the case $p = 1$ features no such occurrence. We will start with a proof in this easier case. The idea is to apply Lemma 6.6 with $M = H_{\infty,L,m,k}$ and $N = H_{\mathcal{M}\cup\{k\}} \setminus H_{\mathcal{M}} = H_{\mathcal{M}\cup\{k\}} \cap \{x \in \mathbb{R}^d : x_k < 0\}$.

We note that these sets satisfy the conditions of Lemma 6.6 with the function φ given by $\varphi(x) := x_k$. Therefore, it remains to estimate the integral

$$\begin{aligned}\int_M \frac{1}{(1+\varphi(x)^2)^{\frac{d}{2}}}\,\mathrm{d}x &= \int_{\mathbb{R}_+^m\times[0,L]^{d-m}\cap\{x\in\mathbb{R}^d:\ \forall j\in\{1,\dots,m\}:\ x_k\geqslant x_j\}} \frac{1}{(1+x_k^2)^{\frac{d}{2}}}\,\mathrm{d}x\\ &= L^{d-m}\int_0^\infty \frac{x_k^{m-1}}{(1+x_k^2)^{\frac{d}{2}}}\,\mathrm{d}x_k\\ &\leqslant L^{d-m}\Big(\int_0^1 x_k^{m-1}\,\mathrm{d}x_k + \int_1^\infty x_k^{m-d-1}\,\mathrm{d}x_k\Big) = L^{d-m}\Big(\frac{1}{m}+\frac{1}{d-m}\Big), \end{aligned}\tag{6.89}$$

where we used that φ is non-negative and measurable as well as Tonelli's theorem. Therefore, Lemma 6.6 yields

$$\|\mathbf{1}_{H_{\infty,L,m,k}}X\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}\setminus H_{\mathcal{M}}}\|_2 \leqslant CL^{\frac{d-m}{2}},\tag{6.90}$$

where the constant $C>0$ does not depend on L. This proves (6.87) for $p=1$.

We now turn to the case $p\geqslant 2$. For each of the $p-1$ occurrences of the projection $\mathbf{1}_{H_{\mathcal{M}}}$, we will subdivide the corresponding subspace $H_{\mathcal{M}}$ into two parts. To do so, we define the following set, for a given measurable function $\phi : [0,\infty[\,\to[0,\infty[$,

$$\begin{aligned}H_\phi := H_{L,m,k,\mathcal{M},\phi} :=&\{x\in\mathbb{R}^d:\ \forall j\in\{1,\dots,m\}\setminus\{k\}: \phi(|x_k|)+|x_k|\geqslant|x_j|\}\\ &\cap\{x\in\mathbb{R}^d:\ \forall j\in\{m+1,\dots,d\}: \phi(|x_k|)+L\geqslant|x_j|\}\cap H_{\mathcal{M}}.\end{aligned}\tag{6.91}$$

For the remaining part of the proof, we set $\varepsilon := \frac{1}{d^p}$. For $l\in\{1,\dots,p-1\}$, we choose the functions $\phi_l : [0,\infty[\,\to[0,\infty[$ given by

$$\phi_l(x) := \tfrac{l}{p}x^{1-\left(\frac{d-m}{d}\right)^l+\varepsilon}\tag{6.92}$$

and note that we have $1-(\frac{d-m}{d})^l+\varepsilon<1$ for all $l\in\{1,\dots,p-1\}$. We start with the first occurrence of $\mathbf{1}_{H_{\mathcal{M}}}$ (from the left) and write $\mathbf{1}_{H_{\mathcal{M}}} = \mathbf{1}_{H_{\phi_1}}+\mathbf{1}_{H_{\mathcal{M}}\setminus H_{\phi_1}}$. We first prove that the operator $\mathbf{1}_{H_{\infty,L,m,k}}X\mathbf{1}_{H_{\mathcal{M}}\setminus H_{\phi_1}}$ is Hilbert-Schmidt. To do so, we apply Lemma 6.6 with $M=H_{\infty,L,m,k}$ and $N=H_{\mathcal{M}}\setminus H_{\phi_1}$. We check that these sets satisfy the conditions of Lemma 6.6 with the function φ given by $\varphi(x) = 1_{\{x_k\geqslant1\}}\frac{1}{3}\phi_1(x_k)$. To see this, let $x\in M$ with $x_k\geqslant 1$ be fixed and let $y\in B_{\varphi(x)}(x)\cap H_{\mathcal{M}}$ be arbitrary. It suffices to show that $y\in H_{\phi_1}$. As $y\in B_{\varphi(x)}(x)$, we obtain the following bound for y_k

$$y_k\geqslant x_k-\tfrac{1}{3p}x_k^{1-\frac{d-m}{d}+\varepsilon}\geqslant x_k\tfrac{3p-1}{3p}.\tag{6.93}$$

Together with the monotonicity of ϕ_1, a bound for $\phi_1(y_k)$ follows

$$\phi_1(y_k)\geqslant\phi_1\big(x_k\tfrac{3p-1}{3p}\big)\geqslant\tfrac{1}{p}\tfrac{3p-1}{3p}x_k^{1-\frac{d-m}{d}+\varepsilon} = \tfrac{3p-1}{3p^2}x_k^{1-\frac{d-m}{d}+\varepsilon}\geqslant\tfrac{2}{3}\phi_1(x_k).\tag{6.94}$$

For each $j\in\{1,\dots,m\}\setminus\{k\}$, we obtain

$$|y_j|\leqslant|x_j|+|y_j-x_j|\leqslant x_k+\tfrac{1}{3}\phi_1(x_k)\leqslant y_k+\tfrac{2}{3}\phi_1(x_k)\leqslant y_k+\phi_1(y_k),\tag{6.95}$$

where we used (6.94) in the last inequality. For $j\in\{m+1,\dots,d\}$, we obtain

$$|y_j|\leqslant|x_j|+|y_j-x_j|\leqslant L+\tfrac{1}{3}\phi_1(x_k)\leqslant L+\phi_1(y_k),\tag{6.96}$$

where we again used (6.94) in the last inequality. Therefore, in order to apply Lemma 6.6, it remains to evaluate the integral

$$\begin{aligned}\int_M \frac{1}{(1+\varphi(x)^2)^{\frac{d}{2}}}\,\mathrm{d}x &= \int_{\mathbb{R}_+^m\times[0,L]^{d-m}\cap\{x\in\mathbb{R}^d:\ \forall j\in\{1,\dots,m\}:\ x_k\geqslant x_j\}} \frac{1}{\left(1+\left(1_{\{x_k\geqslant 1\}}\frac{1}{3}\phi_1(x_k)\right)^2\right)^{\frac{d}{2}}}\,\mathrm{d}x\\ &= L^{d-m}\int_0^\infty \frac{x_k^{m-1}}{\left(1+\left(1_{\{x_k\geqslant 1\}}\frac{1}{3}\phi_1(x_k)\right)^2\right)^{\frac{d}{2}}}\,\mathrm{d}x_k\\ &\leqslant L^{d-m}\Big(\int_0^1 x_k^{m-1}\,\mathrm{d}x_k+\int_1^\infty (3p)^d x_k^{m-m-1-d\varepsilon}\,\mathrm{d}x_k\Big)\leqslant C_1L^{d-m}\frac{p^d}{\varepsilon},\end{aligned}\tag{6.97}$$

where the constant $C_1>0$ is independent of L and p. Therefore, Lemma 6.6 yields

$$\|\mathbf{1}_{H_{\infty,L,m,k}}X\mathbf{1}_{H_{\mathcal{M}}\setminus H_{\phi_1}}\|_2\leqslant C_1'\sqrt{\frac{L^{d-m}p^d}{\varepsilon}},\tag{6.98}$$

with a constant $C_1'>0$ independent of L and p.

We now turn to the intermediate terms, i.e. we show that the operators $\mathbf{1}_{H_{\phi_l}}X\mathbf{1}_{H_{\mathcal{M}}\setminus H_{\phi_{l+1}}}$ are Hilbert-Schmidt for $l\in\{1,\dots,p-2\}$. We again apply Lemma 6.6 with the sets $M=H_{\phi_l}$ and $N=H_{\mathcal{M}}\setminus H_{\phi_{l+1}}$. We show that these sets satisfy the requirements of Lemma 6.6 with the function $\varphi(x)=1_{\{x_k\geqslant 1\}}\frac{1}{2(l+1)p}\phi_{l+1}(x_k)$. To see this, let $x\in H_{\phi_l}$ with $x_k\geqslant 1$ be fixed and let $y\in B_{\varphi(x)}(x)\cap H_{\mathcal{M}}$ be arbitrary. It suffices to show that $y\in H_{\phi_{l+1}}$. As we have $y\in B_{\varphi(x)}(x)$, we obtain the following bound for y_k

$$y_k\geqslant x_k-\tfrac{1}{2p^2}x_k^{1-\left(\frac{d-m}{d}\right)^{l+1}+\varepsilon}\geqslant x_k\tfrac{2p^2-1}{2p^2}.\tag{6.99}$$

Together with the monotonicity of ϕ_{l+1}, we see that

$$\phi_{l+1}(y_k)\geqslant\phi_{l+1}\big(x_k\tfrac{2p^2-1}{2p^2}\big)\geqslant\tfrac{l+1}{p}\tfrac{2p^2-1}{2p^2}\,x_k^{1-\left(\frac{d-m}{d}\right)^{l+1}+\varepsilon}=\tfrac{2lp^2+2p^2-l-1}{2p^3}\,x_k^{1-\left(\frac{d-m}{d}\right)^{l+1}+\varepsilon}.\tag{6.100}$$

As we have $\frac{d-m}{d}\leqslant 1$ and $2p^2-l-1\geqslant 2p$, this yields the following bound

$$\phi_{l+1}(y_k)\geqslant\tfrac{l}{p}\,x_k^{1-\left(\frac{d-m}{d}\right)^{l}+\varepsilon}+\tfrac{1}{p^2}\,x_k^{1-\left(\frac{d-m}{d}\right)^{l+1}+\varepsilon}=\phi_l(x_k)+\tfrac{1}{(l+1)p}\phi_{l+1}(x_k).\tag{6.101}$$

For each $j\in\{1,\dots,m\}\setminus\{k\}$, this yields

$$\begin{aligned}|y_j|&\leqslant|x_j|+|y_j-x_j|\leqslant x_k+\phi_l(x_k)+\tfrac{1}{2(l+1)p}\phi_{l+1}(x_k)\\&\leqslant y_k+\phi_l(x_k)+\tfrac{1}{(l+1)p}\phi_{l+1}(x_k)\leqslant y_k+\phi_{l+1}(y_k),\end{aligned}\tag{6.102}$$

where we used (6.101) in the last inequality. For $j\in\{m+1,\dots,d\}$, we obtain

$$|y_j|\leqslant|x_j|+|y_j-x_j|\leqslant L+\phi_l(x_k)+\tfrac{1}{2(l+1)p}\phi_{l+1}(x_k)\leqslant L+\phi_{l+1}(y_k),\tag{6.103}$$

where we again used (6.101) in the last inequality. Therefore, we have $y\in H_{\phi_{l+1}}$. In order to apply Lemma 6.6, it remains to estimate the integral

$$\int_M\frac{1}{(1+\varphi(x)^2)^{\frac{d}{2}}}\,\mathrm{d}x=\int_{H_{\phi_l}}\frac{1}{\left(1+\left(1_{\{x_k\geqslant 1\}}\frac{1}{2(l+1)p}\phi_{l+1}(x_k)\right)^2\right)^{\frac{d}{2}}}\,\mathrm{d}x.\tag{6.104}$$

We note that $x_k + \phi_l(x_k) \leqslant 2x_k$. By the definition of the set H_{ϕ_l} the right-hand side of (6.104) is bounded from above by

$$2^d \int_{[0,2x_k]^{k-1}\times\mathbb{R}_+\times[0,2x_k]^{m-k}\times[0,L+\phi_l(x_k)]^{d-m}} \frac{1}{\left(1+\left(1_{\{x_k\geqslant 1\}}\frac{1}{2(l+1)p}\phi_{l+1}(x_k)\right)^2\right)^{\frac{d}{2}}}\,\mathrm{d}x$$
$$\leqslant 2^d \int_0^\infty \frac{2^{m-1}x_k^{m-1}\left(L + x_k^{1-\frac{(d-m)^l}{d^l}+\varepsilon}\right)^{d-m}}{\left(1+\left(1_{\{x_k\geqslant 1\}}\frac{1}{2(l+1)p}\phi_{l+1}(x_k)\right)^2\right)^{\frac{d}{2}}}\,\mathrm{d}x_k. \tag{6.105}$$

Splitting the integral on the right-hand side of (6.105) into two parts and applying the definition (6.92) of ϕ_{l+1}, we see that the right-hand side of (6.105) is bounded from above by

$$2^{d+m-1}\left[\int_0^1 x_k^{m-1}2^{d-m}L^{d-m}\,\mathrm{d}x_k\right.$$
$$\left. + \sum_{j=0}^{d-m}\frac{(d-m)!}{j!(d-m-j)!}\int_1^\infty \frac{2^d p^{2d} x_k^{m-1+j-j\frac{(d-m)^l}{d^l}+j\varepsilon}L^{d-m-j}}{x_k^{d-\frac{(d-m)^{l+1}}{d^l}+d\varepsilon}}\,\mathrm{d}x_k\right]$$
$$= 2^{d+m-1}\left[\frac{2^{d-m}L^{d-m}}{m}\right.$$
$$\left. + 2^d p^{2d}\sum_{j=0}^{d-m}\frac{(d-m)!}{j!(d-m-j)!}L^{d-m-j}\int_1^\infty x_k^{-1-(d-m-j)+(d-m-j)\frac{(d-m)^l}{d^l}-(d-j)\varepsilon}\,\mathrm{d}x_k\right]$$
$$\leqslant 2^{d+m-1}\left[\frac{2^{d-m}L^{d-m}}{m} + 2^d p^{2d}\sum_{j=0}^{d-m}\frac{(d-m)!}{j!(d-m-j)!}\frac{L^{d-m-j}}{\varepsilon}\right] \leqslant C_l\frac{p^{2d}L^{d-m}}{\varepsilon}, \tag{6.106}$$

where the constant $C_l > 0$ is independent of L and p. Therefore, Lemma 6.6 yields

$$\|\mathbf{1}_{H_{\phi_l}} X \mathbf{1}_{H_{\mathcal{M}}\setminus H_{\phi_{l+1}}}\|_2 \leqslant C_l'\sqrt{\frac{p^{2d}L^{d-m}}{\varepsilon}}, \tag{6.107}$$

with a constant $C_l' > 0$ independent of L and p.

It remains to show that the remaining operator $\mathbf{1}_{H_{\phi_{p-1}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}\setminus H_{\mathcal{M}}}$ is Hilbert-Schmidt. As before, we do this by an application of Lemma 6.6. We note that the sets $M = H_{\phi_{p-1}}$ and $N = H_{\mathcal{M}\cup\{k\}}\setminus H_{\mathcal{M}} = H_{\mathcal{M}\cup\{k\}}\cap\{x\in\mathbb{R}^d : x_k < 0\}$ satisfy the requirements of Lemma 6.6 with the function $\varphi(x) = x_k$. Again we need to evaluate the corresponding integral

$$\int_{H_{\phi_{p-1}}} \frac{1}{(1+x_k^2)^{\frac{d}{2}}}\,\mathrm{d}x$$
$$= 2^{d-m+|\mathcal{M}|}\int_{[0,x_k+\phi_{p-1}(x_k)]^{k-1}\times\mathbb{R}_+\times[0,x_k+\phi_{p-1}(x_k)]^{m-k}\times[0,L+\phi_{p-1}(x_k)]^{d-m}} \frac{1}{(1+x_k^2)^{\frac{d}{2}}}\,\mathrm{d}x. \tag{6.108}$$

The right-hand side of (6.108) is bounded from above by

$$
\begin{aligned}
&2^d \int_0^\infty \frac{2^{m-1} x_k^{m-1} \Big(L + x_k^{1-\left(\frac{d-m}{d}\right)^{p-1}+\varepsilon}\Big)^{d-m}}{(1+x_k^2)^{\frac{d}{2}}} \,\mathrm{d}x_k \\
&\leqslant 2^{d+m-1} \Bigg[\int_0^1 x_k^{m-1} 2^{d-m} L^{d-m} \,\mathrm{d}x_k \\
&\qquad + \sum_{j=0}^{d-m} \frac{(d-m)!}{j!(d-m-j)!} L^{d-m-j} \int_1^\infty x_k^{-1-(d-m-j)-j\left(\frac{d-m}{d}\right)^{p-1}+j\varepsilon} \,\mathrm{d}x_k \Bigg] \\
&\leqslant 2^{d+m-1} \Big[\frac{2^{d-m} L^{d-m}}{m} + \sum_{j=0}^{d-m} \frac{(d-m)!}{j!(d-m-j)!} \frac{L^{d-m-j}}{\varepsilon} \Big] \leqslant C_{p-1} \sqrt{\frac{L^{d-m}}{\varepsilon}},
\end{aligned} \tag{6.109}
$$

with a constant $C_{p-1} > 0$ independent of L and p. Therefore, Lemma 6.6 yields

$$
\|\mathbf{1}_{H_{\phi_{p-1}}} \mathbf{1}_{H_{\mathcal{M}\cup\{k\}} \setminus H_{\mathcal{M}}}\|_2 \leqslant C'_{p-1} \sqrt{\frac{L^{d-m}}{\varepsilon}}, \tag{6.110}
$$

with a constant $C'_{p-1} > 0$ independent of L and p. Repeated use of the triangle inequality, followed by Hölder's inequality, yields

$$
\begin{aligned}
&\|\mathbf{1}_{H_{\infty,L,m,k}} (\mathbf{1}_{H_{\mathcal{M}}} X)^p (\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} - \mathbf{1}_{H_{\mathcal{M}}})\|_2 \\
&\leqslant \sum_{l=0}^{p-2} \Big\| \mathbf{1}_{H_{\infty,L,m,k}} \Big(\prod_{j=1}^{l} X \mathbf{1}_{H_{\phi_j}} \Big) X \mathbf{1}_{H_{\mathcal{M}} \setminus H_{\phi_{l+1}}} (X \mathbf{1}_{H_{\mathcal{M}}})^{p-2-l} X (\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} - \mathbf{1}_{H_{\mathcal{M}}}) \Big\|_2 \\
&\quad + \Big\| \mathbf{1}_{H_{\infty,L,m,k}} \Big(\prod_{j=1}^{p-1} X \mathbf{1}_{H_{\phi_j}} \Big) X (\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} - \mathbf{1}_{H_{\mathcal{M}}}) \Big\|_2 \\
&\leqslant \|X\|^{p-1} \Big(\|\mathbf{1}_{H_{\infty,L,m,k}} X \mathbf{1}_{H_{\mathcal{M}} \setminus H_{\phi_1}}\|_2 + \sum_{l=1}^{p-2} \|\mathbf{1}_{H_{\phi_l}} X \mathbf{1}_{H_{\mathcal{M}} \setminus H_{\phi_{l+1}}}\|_2 + \|\mathbf{1}_{H_{\phi_{p-1}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}} \setminus H_{\mathcal{M}}}\|_2 \Big) \\
&\leqslant C \|X\|^{p-1} p \sqrt{\frac{p^{2d} L^{d-m}}{\varepsilon}} \leqslant C \|X\|^{p-1} d^{\frac{p}{2}} p^{d+1} L^{\frac{d-m}{2}},
\end{aligned} \tag{6.111}
$$

where we combined estimates (6.98), (6.107) and (6.110) and used the definition of ε in the last line. This proves (6.87) for $p \geqslant 2$.

We continue with the proof of (6.88). The proof works in a similar fashion to the one of (6.87), although it is a bit more involved. We require different partitions of the set $H_{\mathcal{M}}$ as well as different functions ϕ_l, $l \in \{1, \ldots, p-1\}$. Before we define them, we again give a proof in the easier case $p = 1$. We apply Lemma 6.6 with the sets $M = H_{\infty,L,m,k} \setminus H_{L,m,k}$ and $N = H_{\mathcal{M}\cup\{k\}} \setminus H_{\mathcal{M}} = \{x \in H_{\mathcal{M}\cup\{k\}} : \ x_k < 0\}$. These sets fulfil the requirements of Lemma 6.6 with the function $\varphi(x) = x_k$ and we compute

$$
\begin{aligned}
\int_M \frac{1}{(1+\varphi(x)^2)^{\frac{d}{2}}} \,\mathrm{d}x &= \int_{[0,x_k[^{k-1} \times [L,\infty[\times [0,x_k[^{m-k} \times [0,L]^{d-m}} \frac{1}{(1+x_k^2)^{\frac{d}{2}}} \,\mathrm{d}x \\
&= L^{d-m} \int_L^\infty \frac{x_k^{m-1}}{(1+x_k^2)^{\frac{d}{2}}} \,\mathrm{d}x_k \leqslant L^{d-m} \int_L^\infty x_k^{m-d-1} \,\mathrm{d}x_k = \frac{1}{d-m}.
\end{aligned} \tag{6.112}
$$

Then Lemma 6.6 yields the bound (6.88) in the case $p = 1$.

In the case $p \geqslant 2$, we define the sets

$$\begin{aligned} H_{\phi,l} &:= H_{L,m,k,\mathcal{M},p,\phi,l} \\ &:= \{x \in \mathbb{R}^d : \ \forall j \in \{1,\dots,m\} \setminus \{k\} : \phi(|x_k|) + |x_k| \geqslant |x_j|\} \\ &\cap \{x \in \mathbb{R}^d : \ \forall j \in \{m+1,\dots,d\} : \phi(|x_k|) + L \geqslant |x_j|\} \\ &\cap H_{\mathcal{M}} \cap \{x \in \mathbb{R}^d : \ x_k \geqslant \tfrac{p-l}{p} L\}. \end{aligned} \tag{6.113}$$

for a given measurable function $\phi : [0,\infty[\to [0,\infty[$. We recall $\varepsilon = \frac{1}{dp}$. For $l \in \{1,\dots,p-1\}$, we choose the functions $\phi_{l,L} : [0,\infty[\to [0,\infty[$ with

$$\phi_{l,L}(x) := \tfrac{l}{p} L^{\left(\frac{d-m}{d}\right)^l - \varepsilon} \left(\tfrac{p}{p+1-l} x\right)^{1 - \left(\frac{d-m}{d}\right)^l + \varepsilon}. \tag{6.114}$$

We again begin with the first occurrence of $\mathbf{1}_{H_\mathcal{M}}$ (from the left) and write $\mathbf{1}_{H_\mathcal{M}} = \mathbf{1}_{H_{\phi_{1,L},1}} + \mathbf{1}_{H_\mathcal{M} \setminus H_{\phi_{1,L},1}}$. We first prove that the operator $\left(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\right) X \mathbf{1}_{H_\mathcal{M} \setminus H_{\phi_{1,L},1}}$ has its Hilbert-Schmidt norm bounded independently of L. To do so, we apply Lemma 6.6 with $M = H_{\infty,L,m,k} \setminus H_{L,m,k}$ and $N = H_\mathcal{M} \setminus H_{\phi_{1,L},1}$. We check that these sets satisfy the conditions of Lemma 6.6 with the function φ given by $\varphi(x) = \frac{1}{3}\phi_{1,L}(x_k)$. To see this, let $x \in M$ be fixed and let $y \in B_{\varphi(x)}(x) \cap H_\mathcal{M}$ be arbitrary. It suffices to show that $y \in H_{\phi_{1,L},1}$. As $y \in B_{\varphi(x)}(x)$, we obtain the following bound for y_k

$$y_k \geqslant x_k - \tfrac{1}{3p} L^{\frac{d-m}{d} - \varepsilon} x_k^{1 - \frac{d-m}{d} + \varepsilon} \geqslant x_k - \tfrac{1}{3p} x_k = x_k \tfrac{3p-1}{3p}, \tag{6.115}$$

where we used $x_k \geqslant L \geqslant 1$ (as $x \in M$) in the last inequality. In particular we have

$$y_k \geqslant x_k \tfrac{3p-1}{3p} \geqslant \tfrac{3p-1}{3p} L \geqslant \tfrac{p-1}{p} L. \tag{6.116}$$

With the monotonicity of $\phi_{1,L}$, we obtain the following bound for $\phi_{1,L}(y_k)$

$$\phi_{1,L}(y_k) \geqslant \phi_{1,L}\left(x_k \tfrac{3p-1}{3p}\right) \geqslant \tfrac{1}{p} \tfrac{3p-1}{3p} L^{\frac{d-m}{d} - \varepsilon} x_k^{1 - \frac{d-m}{d} + \varepsilon} = \tfrac{3p-1}{3p} \phi_{1,L}(x_k) \geqslant \tfrac{2}{3} \phi_{1,L}(x_k). \tag{6.117}$$

For each $j \in \{1,\dots,m\} \setminus \{k\}$, we obtain

$$|y_j| \leqslant |x_j| + |y_j - x_j| \leqslant x_k + \tfrac{1}{3}\phi_{1,L}(x_k) \leqslant y_k + \tfrac{2}{3}\phi_{1,L}(x_k) \leqslant y_k + \phi_{1,L}(y_k), \tag{6.118}$$

where we used (6.117) in the last inequality. For $j \in \{m+1,\dots,d\}$, we obtain

$$|y_j| \leqslant |x_j| + |y_j - x_j| \leqslant L + \tfrac{1}{3}\phi_{1,L}(x_k) \leqslant L + \phi_{1,L}(y_k), \tag{6.119}$$

where we again used (6.117) in the last inequality. Therefore, in order to apply Lemma 6.6, it remains to evaluate the integral

$$\begin{aligned} \int_M \frac{1}{(1+\varphi(x)^2)^{\frac{d}{2}}} \, \mathrm{d}x &= \int_{[0,x_k[^{k-1} \times [L,\infty[\times [0,x_k[^{m-k} \times [0,L]^{d-m}} \frac{1}{\left(1 + \left(\frac{1}{3}\phi_{1,L}(x_k)\right)^2\right)^{\frac{d}{2}}} \, \mathrm{d}x \\ &= L^{d-m} \int_L^\infty \frac{x_k^{m-1}}{\left(1 + \left(\frac{1}{3}\phi_{1,L}(x_k)\right)^2\right)^{\frac{d}{2}}} \, \mathrm{d}x_k \\ &\leqslant L^{d-m} \int_L^\infty (3p)^d L^{m-d+d\varepsilon} x_k^{m-m-1-d\varepsilon} \, \mathrm{d}x_k \leqslant C_1 \frac{L^{d\varepsilon}}{L^{d\varepsilon}} \frac{p^d}{\varepsilon} = C_1 \frac{p^d}{\varepsilon}, \end{aligned} \tag{6.120}$$

where the constant $C_1 > 0$ is independent of L and p. Therefore, Lemma 6.6 yields

$$\|\left(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\right) X \mathbf{1}_{H_\mathcal{M} \setminus H_{\phi_{1,L},1}}\|_2 \leqslant C_1' \sqrt{\frac{p^d}{\varepsilon}} \tag{6.121}$$

with a constant $C_1' > 0$ independent of L and p.

We again turn towards the intermediate terms, i.e. we show that the operators $\mathbf{1}_{H_{\phi_{l,L},l}} X \mathbf{1}_{H_{\mathcal{M}} \setminus H_{\phi_{l+1,L},l+1}}$ have their Hilbert-Schmidt norm bounded independently of L, for $l \in \{1, \dots, p-2\}$. We again apply Lemma 6.6 with the sets $M = H_{\phi_{l,L},l}$ and $N = H_{\mathcal{M}} \setminus H_{\phi_{l+1,L},l+1}$. We show that these sets satisfy the requirements of Lemma 6.6 with the function $\varphi(x) = \frac{1}{2(l+1)p}\phi_{l+1,L}(x_k)$. To see this, let $x \in H_{\phi_{l,L},l}$ be fixed and let $y \in B_{\varphi(x)}(x) \cap H_{\mathcal{M}}$ be arbitrary. It suffices to show that $y \in H_{\phi_{l+1,L},l+1}$. As $y \in B_{\varphi(x)}(x)$, we get the following bound for y_k

$$\begin{aligned} y_k &\geqslant x_k - \tfrac{1}{2p^2} L^{\left(\frac{d-m}{d}\right)^{l+1}-\varepsilon} \left(\tfrac{p}{p+1-l-1}x_k\right)^{1-\left(\frac{d-m}{d}\right)^{l+1}+\varepsilon} \\ &\geqslant x_k - \tfrac{1}{2p^2}\left(\tfrac{p}{p-l}x_k\right)^{\left(\frac{d-m}{d}\right)^{l+1}-\varepsilon}\left(\tfrac{p}{p-l}x_k\right)^{1-\left(\frac{d-m}{d}\right)^{l+1}+\varepsilon} = x_k \tfrac{2p(p-l)-1}{2p(p-l)}, \end{aligned} \tag{6.122}$$

where we used $\frac{p}{p-l}x_k \geqslant L$ (as $x \in M$) in the last inequality. In particular, we obtain

$$y_k \geqslant x_k \tfrac{2p(p-l)-1}{2p(p-l)} \geqslant \tfrac{p-l}{p}\tfrac{2p(p-l)-1}{2p(p-l)} L = \tfrac{2p^2-2pl-1}{2p^2} L \geqslant \tfrac{p-(l+1)}{p} L. \tag{6.123}$$

With the monotonicity of $\phi_{l+1,L}$, we have

$$\phi_{l+1}(y_k) \geqslant \phi_{l+1}\left(x_k \tfrac{2p(p-l)-1}{2p(p-l)}\right) \geqslant \tfrac{l+1}{p}\tfrac{2p(p-l)-1}{2p(p-l)} L^{\left(\frac{d-m}{d}\right)^{l+1}-\varepsilon}\left(\tfrac{p}{p-l}x_k\right)^{1-\left(\frac{d-m}{d}\right)^{l+1}+\varepsilon}, \tag{6.124}$$

which is bounded from below by

$$\begin{aligned} &\tfrac{2lp(p-l)+2(p-l)}{2p^2(p-l)} L^{\left(\frac{d-m}{d}\right)^{l+1}-\varepsilon}\left(\tfrac{p}{p-l}x_k\right)^{1-\left(\frac{d-m}{d}\right)^{l+1}+\varepsilon} \\ &\quad = \tfrac{l}{p} L^{\left(\frac{d-m}{d}\right)^{l+1}-\varepsilon}\left(\tfrac{p}{p-l}x_k\right)^{1-\left(\frac{d-m}{d}\right)^{l}+\varepsilon}\left(\tfrac{p}{p-l}x_k\right)^{\left(\frac{d-m}{d}\right)^{l}-\left(\frac{d-m}{d}\right)^{l+1}} + \tfrac{1}{(l+1)p}\phi_{l+1,L}(x_k). \end{aligned} \tag{6.125}$$

Using the fact that $\frac{p}{p-l}x_k \geqslant L$, as $x \in H_{\phi_{l,L},l}$, we see that the first term on the right-hand side of (6.125) is bounded from below by

$$\tfrac{l}{p} L^{\left(\frac{d-m}{d}\right)^{l+1}-\varepsilon}\left(\tfrac{p}{p+1-l}x_k\right)^{1-\left(\frac{d-m}{d}\right)^{l}+\varepsilon} L^{\left(\frac{d-m}{d}\right)^{l}-\left(\frac{d-m}{d}\right)^{l+1}} = \phi_{l,L}(x_k). \tag{6.126}$$

This in turn yields the bound

$$\phi_{l+1}(y_k) \geqslant \phi_{l,L}(x_k) + \tfrac{1}{(l+1)p}\phi_{l+1,L}(x_k). \tag{6.127}$$

Therefore, for each $j \in \{1, \dots, m\} \setminus \{k\}$, we obtain

$$\begin{aligned} |y_j| &\leqslant |x_j| + |y_j - x_j| \leqslant x_k + \phi_{l,L}(x_k) + \tfrac{1}{2(l+1)p}\phi_{l+1,L}(x_k) \\ &\leqslant y_k + \phi_{l,L}(x_k) + \tfrac{1}{(l+1)p}\phi_{l+1,L}(x_k) \leqslant y_k + \phi_{l+1,L}(y_k), \end{aligned} \tag{6.128}$$

where we used (6.127) in the last inequality. For $j \in \{m+1, \dots, d\}$, we obtain

$$|y_j| \leqslant |x_j| + |y_j - x_j| \leqslant L + \phi_{l,L}(x_k) + \tfrac{1}{2(l+1)p}\phi_{l+1,L}(x_k) \leqslant L + \phi_{l+1,L}(y_k), \tag{6.129}$$

where we again used (6.127) in the last inequality. Before we are ready to evaluate the integral for Lemma 6.6, we note that for every $x \in H_{\phi_{l,L},l}$ and $l \in \{1, \dots, p-2\}$ we have

$$\begin{aligned} x_k + \phi_{l,L}(x_k) &= x_k + \tfrac{l}{p} L^{\left(\frac{d-m}{d}\right)^{l}-\varepsilon}\left(\tfrac{p}{p+1-l}x_k\right)^{1-\left(\frac{d-m}{d}\right)^{l}+\varepsilon} \\ &\leqslant x_k + \tfrac{l}{p}\left(\tfrac{p}{p-l}x_k\right)^{\left(\frac{d-m}{d}\right)^{l}-\varepsilon}\left(\tfrac{p}{p+1-l}x_k\right)^{1-\left(\frac{d-m}{d}\right)^{l}+\varepsilon} \leqslant x_k + \tfrac{l}{p-l}x_k = \tfrac{p}{p-l}x_k, \end{aligned} \tag{6.130}$$

where we used $\frac{p}{p-l}x_k \geqslant L$. With this at hand, it remains to bound the integral

$$\int_M \frac{1}{(1+\varphi(x)^2)^{\frac{d}{2}}}\,\mathrm{d}x = \int_{H_{\phi_{l,L},l}} \frac{1}{\left(1+\left(\frac{1}{2(l+1)p}\phi_{l+1,L}(x_k)\right)^2\right)^{\frac{d}{2}}}\,\mathrm{d}x \tag{6.131}$$

in order to apply Lemma 6.6. By the definition of $H_{\phi_{l,L},l}$ and (6.130), the right-hand side of (6.131) is bounded from above by

$$2^d \int_{\left[0,\frac{p}{p-l}x_k\right]^{k-1}\times\left[\frac{p-l}{p}L,\infty\right[\times\left[0,\frac{p}{p-l}x_k\right]^{m-k}\times[0,L+\phi_{l,L}(x_k)]^{d-m}} \frac{1}{\left(\frac{1}{2(l+1)p}\phi_{l+1,L}(x_k)\right)^d}\,\mathrm{d}x$$

$$= 2^d \int_{\frac{p-l}{p}L}^{\infty} \frac{\left(\frac{p}{p-l}x_k\right)^{m-1}\left(L+\frac{l}{p}L^{\left(\frac{d-m}{d}\right)^l-\varepsilon}\left(\frac{p}{p+1-l}x_k\right)^{1-\left(\frac{d-m}{d}\right)^l+\varepsilon}\right)^{d-m}}{\left(\frac{1}{2(l+1)p}\phi_{l+1,L}(x_k)\right)^d}\,\mathrm{d}x_k. \tag{6.132}$$

As $\frac{p}{p-l}x_k \geqslant L$, this is in turn bounded from above by

$$2^{2d-m}\int_{\frac{p-l}{p}L}^{\infty} \frac{\left(\frac{p}{p-l}x_k\right)^{m-1}\left(L^{\left(\frac{d-m}{d}\right)^l-\varepsilon}\left(\frac{p}{p-l}x_k\right)^{1-\left(\frac{d-m}{d}\right)^l+\varepsilon}\right)^{d-m}}{\left(\frac{1}{2(l+1)p}\phi_{l+1,L}(x_k)\right)^d}\,\mathrm{d}x_k. \tag{6.133}$$

Using the definition of $\phi_{l+1,L}$, this is equal to

$$2^{3d-m}p^{2d}\int_{\frac{p-l}{p}L}^{\infty} \frac{\left(\frac{p}{p-l}x_k\right)^{m-1} L^{\frac{(d-m)^{l+1}}{d^l}-(d-m)\varepsilon}\left(\frac{p}{p-l}x_k\right)^{d-m-\frac{(d-m)^{l+1}}{d^l}+(d-m)\varepsilon}}{L^{\frac{(d-m)^{l+1}}{d^l}-d\varepsilon}\left(\frac{p}{p-l}x_k\right)^{d-\frac{(d-m)^{l+1}}{d^l}+d\varepsilon}}\,\mathrm{d}x_k$$

$$= 2^{3d-m}p^{2d}\int_{\frac{p-l}{p}L}^{\infty} L^{m\varepsilon}\left(\frac{p}{p-l}x_k\right)^{-1-m\varepsilon}\,\mathrm{d}x_k. \tag{6.134}$$

Carrying out the integration, we see that the right-hand side of (6.131) bounded from above by

$$2^{3d-m}p^{2d}L^{m\varepsilon-m\varepsilon}\tfrac{1}{m\varepsilon} \leqslant C_l\frac{p^{2d}}{\varepsilon}, \tag{6.135}$$

where the constant $C_l > 0$ is independent of L and p. Therefore, Lemma 6.6 yields

$$\|\mathbf{1}_{H_{\phi_l}}X\mathbf{1}_{H_{\mathcal{M}}\setminus H_{\phi_{l+1}}}\|_2 \leqslant C_l'\sqrt{\frac{p^{2d}}{\varepsilon}} \tag{6.136}$$

with a constant $C_l' > 0$ independent of L and p.

It again remains to show that the remaining operator $\mathbf{1}_{H_{\phi_{p-1,L},p-1}}X\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}\setminus H_{\mathcal{M}}}$ has Hilbert-Schmidt norm bounded independently of L. As before, we do this by an application of Lemma 6.6. We note that the sets $M = H_{\phi_{p-1,L},p-1}$ and $N = H_{\mathcal{M}\cup\{k\}}\setminus H_{\mathcal{M}} = H_{\mathcal{M}\cup\{k\}}\cap\{x\in\mathbb{R}^d : x_k < 0\}$ satisfy the requirements of Lemma 6.6 with the function $\varphi(x) = x_k$. With the definition of $H_{\phi_{p-1,L},p-1}$, the corresponding integral reads

$$\int_M \frac{1}{(1+\varphi(x)^2)^{\frac{d}{2}}}\,\mathrm{d}x = \int_{H_{\phi_{p-1,L},p-1}} \frac{1}{(1+x_k^2)^{\frac{d}{2}}}\,\mathrm{d}x$$

$$= 2^{d-m+|\mathcal{M}|}\int_{[0,x_k+\phi_{p-1,L}(x_k)]^{k-1}\times\left[\frac{L}{p},\infty\right[\times[0,x_k+\phi_{p-1,L}(x_k)]^{m-k}\times[0,L+\phi_{p-1,L}(x_k)]^{d-m}} \frac{1}{(1+x_k^2)^{\frac{d}{2}}}\,\mathrm{d}x. \tag{6.137}$$

With the help of (6.130), the right-hand side of (6.137) is bounded from above by

$$2^{2d-m}\int_{\frac{L}{p}}^{\infty}\frac{(px_k)^{m-1}\Big(L^{\left(\frac{d-m}{d}\right)^{p-1}-\varepsilon}(px_k)^{1-\left(\frac{d-m}{d}\right)^{p-1}+\varepsilon}\Big)^{d-m}}{x_k^d}\,\mathrm{d}x_k$$
$$\leqslant 2^{2d-m}p^{d-1}\int_{\frac{L}{p}}^{\infty}L^{\frac{(d-m)^p}{d^{p-1}}-(d-m)\varepsilon}x_k^{-1-\frac{(d-m)^p}{d^{p-1}}+(d-m)\varepsilon}\,\mathrm{d}x_k. \quad (6.138)$$

Carrying out the integration, we obtain the bound

$$\int_M\frac{1}{(1+\varphi(x)^2)^{\frac{d}{2}}}\,\mathrm{d}x\leqslant C_{p-1}\frac{p^{d-1}}{\varepsilon}, \quad (6.139)$$

with a constant $C_{p-1}>0$ independent of L and p. Therefore, Lemma 6.6 yields

$$\|\mathbf{1}_{H_{\phi_{p+1}}}X\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}\setminus H_{\mathcal{M}}}\|_2\leqslant C'_{p-1}\sqrt{\frac{p^{d-1}}{\varepsilon}}, \quad (6.140)$$

with a constant $C'_{p-1}>0$ independent of L and p. The proof of (6.88) follows in the same manner as the proof (6.87): We first estimate

$$\Big\|\big(\mathbf{1}_{H_{\infty,L,m,k}}-\mathbf{1}_{H_{L,m,k}}\big)(\mathbf{1}_{H_{\mathcal{M}}}X)^p(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}-\mathbf{1}_{H_{\mathcal{M}}})\Big\|_2$$
$$\leqslant\sum_{l=0}^{p-2}\Big\|\big(\mathbf{1}_{H_{\infty,L,m,k}}-\mathbf{1}_{H_{L,m,k}}\big)\Big(\prod_{j=1}^{l}X\mathbf{1}_{H_{\phi_{j,L},j}}\Big)X\mathbf{1}_{H_{\mathcal{M}}\setminus H_{\phi_{l+1,L},l+1}}(X\mathbf{1}_{H_{\mathcal{M}}})^{p-2-l}X(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}-\mathbf{1}_{H_{\mathcal{M}}})\Big\|_2$$
$$+\Big\|\big(\mathbf{1}_{H_{\infty,L,m,k}}-\mathbf{1}_{H_{L,m,k}}\big)\Big(\prod_{j=1}^{p-1}X\mathbf{1}_{H_{\phi_{j,L},j}}\Big)X(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}-\mathbf{1}_{H_{\mathcal{M}}})\Big\|_2 \quad (6.141)$$

which in turn is bounded from above by

$$\|X\|^{p-1}\Big[\Big\|\big(\mathbf{1}_{H_{\infty,L,m,k}}-\mathbf{1}_{H_{L,m,k}}\big)X\mathbf{1}_{H_{\mathcal{M}}\setminus H_{\phi_{1,L},1}}\Big\|_2$$
$$+\sum_{l=1}^{p-2}\big\|\mathbf{1}_{H_{\phi_{l,L},l}}X\mathbf{1}_{H_{\mathcal{M}}\setminus H_{\phi_{l+1,L},l+1}}\big\|_2+\big\|\mathbf{1}_{H_{\phi_{p-1,L},p-1}}X\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}\setminus H_{\mathcal{M}}}\big\|_2\Big]$$
$$\leqslant C'\|X\|^{p-1}p\sqrt{\frac{p^{2d}}{\varepsilon}}\leqslant C'\|X\|^{p-1}d^{\frac{p}{2}}p^{d+1}, \quad (6.142)$$

where we combined estimates (6.121), (6.136) and (6.140) and used the definition of ε in the last line. This proves (6.88) for $p\geqslant 2$ and concludes the proof of the lemma. □

We now use the just obtained Hilbert-Schmidt estimate, to derive a trace norm estimate for monomial test functions.

Lemma 6.12. *Let X be a bounded integral operator whose kernel satisfies the bound* (6.15). *Let $1\leqslant k\leqslant m<d$ and $\mathcal{M}\subseteq\{1,\dots,m\}$ such that $k\notin\mathcal{M}$. Let $L\geqslant 1$ and $p\in\mathbb{N}$. Then the operator*

$$\mathbf{1}_{H_{\infty,L,m,k}}\big[(\mathbf{1}_{H_{\mathcal{M}}}X\mathbf{1}_{H_{\mathcal{M}}})^p-(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}X\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}})^p\big]\mathbf{1}_{H_{\infty,L,m,k}} \quad (6.143)$$

is trace class and there exists a constant $C>0$, independent of L and p, such that

$$\Big\|\mathbf{1}_{H_{\infty,L,m,k}}\big[(\mathbf{1}_{H_{\mathcal{M}}}X\mathbf{1}_{H_{\mathcal{M}}})^p-(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}X\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}})^p\big]\mathbf{1}_{H_{\infty,L,m,k}}\Big\|_1$$
$$\leqslant CL^{d-m}\|X\|^{p-1}(2d)^{p-1}(p-1)^{2d+2}. \quad (6.144)$$

Furthermore, there exists a constant $C' > 0$ which is independent of L and p such that

$$\begin{aligned}\Big\|\big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big)\big[\big(\mathbf{1}_{H_{\mathcal{M}}}X\mathbf{1}_{H_{\mathcal{M}}}\big)^p - \big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}X\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)^p\big]\big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big)\Big\|_1 \\ \leqslant C'\|X\|^{p-1}\big(2d\big)^{p-1}(p-1)^{2d+2}. \quad (6.145)\end{aligned}$$

Proof. We start by proving (6.144). The proof works in a similar way as the proof of Lemma 6.10. Set $P_0 := \mathbf{1}_{H_{\mathcal{M}}}$ and $P_1 := \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}$. Using the fact that $\mathbf{1}_{H_{\infty,L,m,k}}P_0 = \mathbf{1}_{H_{\infty,L,m,k}}P_1 = \mathbf{1}_{H_{\infty,L,m,k}}$, we rewrite the operator (6.143) in the following way

$$\mathbf{1}_{H_{\infty,L,m,k}}\big[\big(XP_0\big)^{p-1} - \big(XP_1\big)^{p-1}\big]X\mathbf{1}_{H_{\infty,L,m,k}} \quad (6.146)$$

and see that in the case $p = 1$ there is nothing to show. If $p \geqslant 2$, we define $P_2 = P_1 - P_0$ and write

$$\begin{aligned}\mathbf{1}_{H_{\infty,L,m,k}}\big(XP_1\big)^{p-1}X\mathbf{1}_{H_{\infty,L,m,k}} &= \mathbf{1}_{H_{\infty,L,m,k}}\big(XP_0 + XP_2\big)^{p-1}X\mathbf{1}_{H_{\infty,L,m,k}} \\ &= \sum_{\pi=(\pi_1,\dots,\pi_{p-1})\in\{0,2\}^{p-1}} \mathbf{1}_{H_{\infty,L,m,k}}\Big(\prod_{j=1}^{p-1} XP_{\pi(j)}\Big)X\mathbf{1}_{H_{\infty,L,m,k}}. \quad (6.147)\end{aligned}$$

With this at hand, we estimate the trace norm of (6.146) by

$$\sum_{\pi\in\{0,2\}^{p-1}:\ \pi\neq 0} \Big\|\mathbf{1}_{H_{\infty,L,m,k}}\Big(\prod_{j=1}^{p-1} XP_{\pi(j)}\Big)X\mathbf{1}_{H_{\infty,L,m,k}}\Big\|_1. \quad (6.148)$$

Each of these trace norms contains at least one factor P_2. Setting $p_{1,\pi} := \min\{j \in \{1,\dots,p-1\} : \pi(j) = 2\}$ and $p_{2,\pi} := \max\{j \in \{1,\dots,p-1\} : \pi(j) = 2\}$ for a given $\pi \in \{0,2\}^{p-1}$ with $\pi \neq 0$, we estimate (6.148) by

$$\sum_{\pi\in\{0,2\}^{p-1}:\ \pi\neq 0} \|X\|^{p-1-p_{1,\pi}-p_{2,\pi}}\Big\|\mathbf{1}_{H_{\infty,L,m,k}}\big(P_0X\big)^{p_{1,\pi}}P_2\Big\|_2\Big\|P_2\big(XP_0\big)^{p_{2,\pi}}\mathbf{1}_{H_{\infty,L,m,k}}\Big\|_2. \quad (6.149)$$

By Lemma 6.11, there exists a constant $C > 0$, independent of L and p, such that (6.149) is bounded by

$$\begin{aligned}CL^{d-m}\|X\|^{p-1} \sum_{\pi\in\{0,2\}^{p-1}:\ \pi\neq 0} d^{\frac{p_{1,\pi}+p_{2,\pi}}{2}}(p_{1,\pi})^{d+1}(p_{2,\pi})^{d+1} \\ \leqslant CL^{d-m}\|X\|^{p-1}\big(2d\big)^{p-1}(p-1)^{2d+2}. \quad (6.150)\end{aligned}$$

This concludes the proof of (6.144). In order to prove (6.145), we use an analogous argument to estimate the left-hand side of (6.145) by

$$\begin{aligned}\sum_{\pi\in\{0,2\}^{p-1}:\ \pi\neq 0} \|X\|^{p-1-p_{1,\pi}-p_{2,\pi}}\Big\|\big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big)\big(P_0X\big)^{p_{1,\pi}}P_2\Big\|_2 \\ \times \Big\|P_2\big(XP_0\big)^{p_{2,\pi}}\big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big)\Big\|_2. \quad (6.151)\end{aligned}$$

Again Lemma 6.11 yields a constant $C' > 0$, independent of L and p, such that (6.151) is bounded by

$$C'\|X\|^{p-1} \sum_{\pi\in\{0,2\}^{p-1}:\ \pi\neq 0} d^{\frac{p_{1,\pi}+p_{2,\pi}}{2}}(p_{1,\pi})^{d+1}(p_{2,\pi})^{d+1} \leqslant C'\|X\|^{p-1}\big(2d\big)^{p-1}(p-1)^{2d+2}. \quad (6.152)$$

This concludes the proof of (6.145). □

It remains to extend this estimate to analytic functions, which we do in the following

Lemma 6.13. *Let X be a bounded integral operator whose kernel satisfies the bound* (6.15). *Let $1 \leqslant k \leqslant m < d$ and $\mathcal{M} \subseteq \{1, \dots, m\}$ such that $k \notin \mathcal{M}$. Let $L \geqslant 1$ and g be an entire function such that $g(0) = 0$. Then the operator*

$$\mathbf{1}_{H_{\infty,L,m,k}}\big[g\big(\mathbf{1}_{H_{\mathcal{M}}}X\mathbf{1}_{H_{\mathcal{M}}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}X\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\big]\mathbf{1}_{H_{\infty,L,m,k}} \tag{6.153}$$

is trace class and there exists a constant $C > 0$, which is independent of L, such that

$$\big\|\big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big)\big[g\big(\mathbf{1}_{H_{\mathcal{M}}}X\mathbf{1}_{H_{\mathcal{M}}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}X\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\big]\big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big)\big\|_1 \leqslant C. \tag{6.154}$$

Proof. We begin by proving (6.153). There exists a natural number $N_0 \in \mathbb{N}$ such that $p^{2d+2} \leqslant 2^p$ for all $p \geqslant N_0$. Using Lemma 6.12, we write

$$\begin{aligned}
&\big\|\mathbf{1}_{H_{\infty,L,m,k}}\big[g\big(\mathbf{1}_{H_{\mathcal{M}}}X\mathbf{1}_{H_{\mathcal{M}}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}X\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\big]\mathbf{1}_{H_{\infty,L,m,k}}\big\|_1 \\
&\qquad = \Big\|\sum_{p=1}^{\infty}\omega_p\big\{\mathbf{1}_{H_{\infty,L,m,k}}\big[\big(\mathbf{1}_{H_{\mathcal{M}}}X\mathbf{1}_{H_{\mathcal{M}}}\big)^p - \big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}X\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)^p\big]\mathbf{1}_{H_{\infty,L,m,k}}\big\}\Big\|_1 \\
&\qquad \leqslant C_1L^{d-m} + C_2L^{d-m}\sum_{p=N_0}^{\infty}|\omega_p|\big(4d\|X\|\big)^{p-1} \leqslant C_3L^{d-m},
\end{aligned} \tag{6.155}$$

with constants $C_1, C_2, C_3 > 0$ independent of L. In order to prove (6.154), we again use Lemma 6.12 to estimate

$$\begin{aligned}
&\big\|\big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big)\big[g\big(\mathbf{1}_{H_{\mathcal{M}}}X\mathbf{1}_{H_{\mathcal{M}}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}X\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\big]\big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big)\big\|_1 \\
&\qquad \leqslant C_4 + C_5\sum_{p=N_0}^{\infty}|\omega_p|\big(4d\|X\|\big)^{p-1} \leqslant C,
\end{aligned} \tag{6.156}$$

with constants $C_4, C_5, C > 0$ independent of L. This concludes the proof of the lemma. □

6.3.3. Proof of Theorem 6.8.

With this at hand, we are now ready to prove Theorem 6.8.

Proof of Theorem 6.8. We start by proving (6.58). The asymptotic expansion (6.59) follows by counting the number of occurring terms. After the localisation in Lemma 6.10, the expansion (6.58) reduces to analysing the trace

$$\sum_{V\in\mathcal{F}^{(0)}}\mathbf{1}_{H_{V,L}}\sum_{m=0}^{d-1}\sum_{F\in\mathcal{F}_V^{(d-m)}}X_{F,g}. \tag{6.157}$$

As explained in the strategy of the proof at the beginning of Section 6.3.2, this analysis, and with it the proof of (6.58), reduces to showing that

$$\begin{aligned}
&\sum_{m=0}^{d-1}\sum_{V\in\mathcal{F}^{(0)}}\sum_{F\in\mathcal{F}_V^{(d-m)}}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\mathbf{1}_{H_{V,L}}X_{F,g}\big] \\
&\qquad = \sum_{m=0}^{d-1}L^{d-m}\lim_{L\to\infty}\sum_{V\in\mathcal{F}^{(0)}}\sum_{F\in\mathcal{F}_V^{(d-m)}}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\mathbf{1}_{H_{F,L,V}}X_{F,g}\big] + O(1),
\end{aligned} \tag{6.158}$$

as $L \to \infty$ (cf. (6.77)). Therefore, we begin by showing that, for a given vertex V and a given $(d-m)$-face F, we have

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\mathbf{1}_{H_{V,L}}X_{F,g}\big] = L^{d-m}\lim_{L\to\infty}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\big[\mathbf{1}_{H_{F,L,V}}X_{F,g}\big] + O(1), \tag{6.159}$$

as $L \to \infty$. After suitable rotation and translation we can again consider the situation with the designated vertex $V = \{0\}$ and $(d-m)$-face $F = \{0\}^m \times [0,2]^{d-m}$. We recall that in this case we have

$$H_{V,L} = [0,L]^d, \quad H_{F,L,V} = [0,L]^m \times [0,1]^{d-m}. \tag{6.160}$$

In the easy case $m = 0$, the operator $X_{F,g} = g(X)$ is translation invariant. It also has continuous kernel on the interior $(H_{F,L,V})^\circ$ of the set $H_{F,L,V}$ by the following lemma, whose proof we postpone for the remaining duration of the proof of Theorem 6.8.

Lemma 6.14. *Let $\Omega \subseteq \mathbb{R}^d$ be open, let X be as in Theorem* 6.8 *and let $g : \mathbb{C} \to \mathbb{C}$ be an entire function. Then the integral kernel of the operator $g\big(\mathbf{1}_\Omega X \mathbf{1}_\Omega\big)$ is continuous on $\Omega \times \Omega$.*

Then (6.159) follows by integrating the kernel of X along the diagonal. In the other cases we apply the results of Section 6.3.2. Let $k \in \{1,\dots,m\}$ and $\mathcal{M} \subseteq \{1,\dots,m\} \setminus \{k\}$ be arbitrary. Comparing the operators (6.82) and (6.83), we first show that

$$\begin{aligned}&\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{H_{L,m,k}}\Big(g\big(\mathbf{1}_{H_\mathcal{M}} X \mathbf{1}_{H_\mathcal{M}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\Big)\Big]\\ &\quad = \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{H_{\infty,L,m,k}}\Big(g\big(\mathbf{1}_{H_\mathcal{M}} X \mathbf{1}_{H_\mathcal{M}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\Big)\mathbf{1}_{H_{\infty,L,m,k}}\Big] + O(1),\end{aligned} \tag{6.161}$$

as $L \to \infty$. The operator

$$\mathbf{1}_{H_{\infty,L,m,k}}\Big(g\big(\mathbf{1}_{H_\mathcal{M}} X \mathbf{1}_{H_\mathcal{M}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\Big)\mathbf{1}_{H_{\infty,L,m,k}} \tag{6.162}$$

is trace class by Lemma 6.13. By the cyclic property of the trace and the fact that $H_{L,m,k} \subset H_{\infty,L,m,k}$, we see that the operators

$$\begin{aligned}&\mathbf{1}_{H_{\infty,L,m,k}}\Big(g\big(\mathbf{1}_{H_\mathcal{M}} X \mathbf{1}_{H_\mathcal{M}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\Big)\mathbf{1}_{H_{\infty,L,m,k}}\\ &\qquad - \mathbf{1}_{H_{L,m,k}}\Big(g\big(\mathbf{1}_{H_\mathcal{M}} X \mathbf{1}_{H_\mathcal{M}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\Big)\end{aligned} \tag{6.163}$$

and

$$\big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big)\Big(g\big(\mathbf{1}_{H_\mathcal{M}} X \mathbf{1}_{H_\mathcal{M}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\Big)\big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big) \tag{6.164}$$

have the same trace. Now, Lemma 6.13 yields a constant $C > 0$, independent of L, such that for all $L \geqslant 1$ we have

$$\Big\|\big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big)\Big(g\big(\mathbf{1}_{H_\mathcal{M}} X \mathbf{1}_{H_\mathcal{M}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\Big)\big(\mathbf{1}_{H_{\infty,L,m,k}} - \mathbf{1}_{H_{L,m,k}}\big)\Big\|_1 \leqslant C. \tag{6.165}$$

As the operators $g\big(\mathbf{1}_{H_\mathcal{M}} X \mathbf{1}_{H_\mathcal{M}}\big)$ and $g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)$ are translation invariant in the last $(d-m)$ variables with continuous kernel, cf. Lemma 6.14, we obtain

$$\begin{aligned}&\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{H_{\infty,L,m,k}}\Big(g\big(\mathbf{1}_{H_\mathcal{M}} X \mathbf{1}_{H_\mathcal{M}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\Big)\mathbf{1}_{H_{\infty,L,m,k}}\Big]\\ &\quad = L^{d-m}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{H_{\infty,1,m,k}}\Big(g\big(\mathbf{1}_{H_\mathcal{M}} X \mathbf{1}_{H_\mathcal{M}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\Big)\mathbf{1}_{H_{\infty,1,m,k}}\Big]\\ &\quad = L^{d-m}\lim_{L\to\infty}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{H_{L,1,m,k}}\Big(g\big(\mathbf{1}_{H_\mathcal{M}} X \mathbf{1}_{H_\mathcal{M}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\Big)\Big],\end{aligned} \tag{6.166}$$

where $H_{\infty,1,m,k} = \{x \in \mathbb{R}_+^m \times [0,1]^{d-m} : \forall j \in \{1,\dots,m\} \setminus \{k\} : x_j \leqslant x_k\}$, $H_{L,1,m,k} := \{x \in [0,L]^m \times [0,1]^{d-m} : \forall j \in \{1,\dots,m\} \setminus \{k\} : x_j \leqslant x_k\}$ and we again used the cyclic property of the trace. The operator

$$\mathbf{1}_{H_{\infty,1,m,k}}\Big(g\big(\mathbf{1}_{H_\mathcal{M}} X \mathbf{1}_{H_\mathcal{M}}\big) - g\big(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}} X \mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\big)\Big)\mathbf{1}_{H_{\infty,1,m,k}} \tag{6.167}$$

is trace class by Lemma 6.13 with $L = 1$.

Combining (6.161) and (6.166), adding the contributions for every $k \in \{1, \dots, m\}$ and $\mathcal{M} \subseteq \{1, \dots, m\} \setminus \{k\}$, as well as reordering the terms, we obtain

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\sum_{k=0}^{m}(-1)^k \sum_{\mathcal{M}\subseteq\{1,\dots,m\}\,:\,|\mathcal{M}|=k} \mathbf{1}_{H_{V,L}}\, g(\mathbf{1}_{H_\mathcal{M}} X \mathbf{1}_{H_\mathcal{M}})\right]$$
$$= L^{d-m} \lim_{L\to\infty} \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\sum_{k=0}^{m}(-1)^k \sum_{\mathcal{M}\subseteq\{1,\dots,m\}\,:\,|\mathcal{M}|=k} \mathbf{1}_{H_{F,L,V}}\, g(\mathbf{1}_{H_\mathcal{M}} X \mathbf{1}_{H_\mathcal{M}})\right] + O(1), \quad (6.168)$$

as $L \to \infty$. Together with (6.79) this yields (6.159) for the designated vertex $V = \{0\}$ and $(d-m)$-face $F = \{0\}^m \times [0,2]^{d-m}$. Rotating and translating back, we obtain (6.159) for an arbitrary vertex V and $(d-m)$-face F. Adding up the contributions of all V and F yields (6.158). Recollecting the contributions of all vertices in F via the equality $H_{F,L} = \sum_{\{V\in\mathcal{F}^{(0)}:V\in F\}} H_{F,L,V}$, finishes the proof of (6.58).

In order to prove (6.59), it just remains to count the number of contributions in (6.58). Clearly we have $\left|\mathcal{F}^{(d-m)}\right| = 2^m \frac{d!}{m!(d-m)!}$ and $\left|\mathcal{F}_F^{(k+(d-m))}\right| = \frac{m!}{k!(m-k)!}$ for a given $(d-m)$-face F and $k \in \{0, \dots, m\}$. The latter corresponds to the number of operators occurring in the definition (6.53) of $X_{F,g}$. Therefore, we obtain the constants $c_{k,m} = 2^m \frac{d!}{m!(d-m)!}(-1)^k \frac{m!}{k!(m-k)!} = \frac{(-1)^k 2^m d!}{k!(m-k)!(d-m)!}$ for $0 \leqslant k \leqslant m \leqslant d$. This concludes the proof of (6.59) and of Theorem 6.8. □

Proof of Lemma 6.14. We prove the lemma for monomials $g(z) = z^p$, $p \in \mathbb{N}$. The extension to entire functions works in the usual way. For $p = 1$ there is nothing to show. The operator $\left(\mathbf{1}_\Omega X \mathbf{1}_\Omega\right)^p$ has integral kernel

$$K_{\Omega,p}(x,y) = \int_\Omega \dots \int_\Omega F_p(x, x_1, \dots, x_{p-1}, y)\, \mathrm{d}x_{p-1} \dots x_1, \quad (6.169)$$

where

$$F_p(x, x_1, \dots, x_{p-1}, y) := K(x, x_1)K(x_1, x_2)\dots K(x_{p-2}, x_{p-1})K(x_{p-1}, y) \quad (6.170)$$

with K being the integral kernel of X. The bound (6.15) implies

$$|F_p(x, x_1, \dots, x_{p-1}, y)| \leqslant C_K^p \frac{1}{(1+|x-x_1|^2)^{\frac{d}{2}}} \cdots \frac{1}{(1+|x_{p-1}-y|^2)^{\frac{d}{2}}}. \quad (6.171)$$

Fix $x_0, x_p \in \Omega$ and $\delta \in]0,1[$ such that $B_\delta(x_0) \times B_\delta(x_p) \subset \Omega \times \Omega$. By Peetre's inequality we have

$$\left(\frac{1+|x-x_1|^2}{1+|x_0-x_1|^2}\right)^{\frac{d}{2}} \leqslant \left(2(1+|x-x_0|^2)\right)^{\frac{d}{2}} < 2^d, \quad (6.172)$$

for all $x \in B_\delta(x_0)$ and $x_1 \in \mathbb{R}^d$, as well as

$$\left(\frac{1+|x_{p-1}-y|^2}{1+|x_{p-1}-x_p|^2}\right)^{\frac{d}{2}} \leqslant \left(2(1+|y-x_p|^2)\right)^{\frac{d}{2}} < 2^d, \quad (6.173)$$

for all $y \in B_\delta(x_p)$ and $x_{p-1} \in \mathbb{R}^d$. In combination with (6.171) the bound

$$\sup_{(x,y)\in B_\delta(x_0)\times B_\delta(y_0)} |F_p(x, x_1, \dots, x_{p-1}, y)| \leqslant 4^d C_K^p \prod_{k=0}^{p-1} \frac{1}{(1+|x_k - x_{k+1}|^2)^{\frac{d}{2}}} \quad (6.174)$$

follows. As the right-hand side of (6.174) is integrable on $\Omega^{p-1} \subseteq (\mathbb{R}^d)^{p-1}$, we infer the continuity of the kernel $K_{\Omega,p}$. □

6.4. Estimates for smooth symbols and an upper bound

In this section we further study the trace of the remaining operator

$$\sum_{V\in\mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}} X_{V,g}. \tag{6.175}$$

From here on, we only consider the special case of the free massless Dirac operator, given by our application, i.e. we set $X = \mathrm{Op}(\psi\mathcal{D})$. As in Section 6.3 we choose a designated vertex $V = V_0 = \{0\}$ such that $H_{V,L} = H_{V_0,L} = [0,L]^d$ and

$$X_g := X_{V_0,g} = \sum_{k=0}^{d}(-1)^k \sum_{\mathcal{M}\subseteq\{1,\dots,d\}\,:\,|\mathcal{M}|=k} g(\mathbf{1}_{H_{\mathcal{M}}}\mathrm{Op}(\psi\mathcal{D})\mathbf{1}_{H_{\mathcal{M}}}), \tag{6.176}$$

where we recall $H_{\mathcal{M}} = \{x\in\mathbb{R}^d : \forall j\in\{1,\dots,d\}\setminus\mathcal{M} : x_j \geqslant 0\}$ from the last section. The other vertices reduce to this case after suitable rotation and translation. In order to derive a logarithmic upper bound for the trace norm of (6.175), we make use of the fact that the symbol $\psi\mathcal{D}$ is discontinuous at a single point, the origin, and is smooth away from it, as well as compactly supported. We follow the usual strategy, for example laid out in [Sob14], to first establish "non-enhanced" bounds for symbols which are both smooth and compactly supported and then to obtain a logarithmically enhanced bound for the discontinuous symbol from there.

The estimate for smooth and compactly supported symbols utilised in this chapter is based on the estimates in [Sob14] and is similar, in the choice of sets and proof, to the result [Pfi19, Cor. 3.7].

Lemma 6.15. *Let $\psi\in\mathbb{C}_c^\infty(\mathbb{R}^d)$ be supported in a ball of radius $\rho>1$ centred about some $\xi_0\in\mathbb{R}^d$. Let $M,N\subset\mathbb{R}^d$ be such that there exists $\beta\geqslant 0$ and a constant $C_\beta>0$ with the property that, for all $r>0$, we have*

$$|\{x\in\mathbb{Z}^d : Q_x\cap M_\rho \neq \emptyset \text{ and } \operatorname{dist}(x,N_\rho)\leqslant r\}| \leqslant C_\beta(1+r^2)^{\frac{\beta}{2}}, \tag{6.177}$$

where Q_x is the closed unit cube centred about x, and M_ρ respectively N_ρ are the scaled versions of the respective sets. Then the operator $M\,\mathrm{Op}(\psi\otimes\mathbb{1}_n)N$ is trace class and there exists a constant $C>0$, which is independent of ρ, M and N, such that

$$\|\mathbf{1}_M\,\mathrm{Op}(\psi\otimes\mathbb{1}_n)\mathbf{1}_N\|_1 \leqslant C_\beta C \max_{|\alpha|\leqslant 2d+\beta+1}\sup_{\xi\in\mathbb{R}^d}\rho^{|\alpha|}|\partial_\xi^\alpha\psi(\xi)|, \tag{6.178}$$

where $|\alpha| := \sum_{k=1}^d \alpha_k$ for a given multi-index $\alpha\in\mathbb{N}_0^d$.

Proof. By the unitary dilatation U_ρ on $L^2(\mathbb{R}^d)\otimes\mathbb{C}^n$, with $(U_\rho u)(x) := \rho^{\frac{d}{2}}u(\rho x)$ for all $u\in L^2(\mathbb{R}^d)\otimes\mathbb{C}^n$, the operator $\mathbf{1}_M\,\mathrm{Op}(\psi\otimes\mathbb{1}_n)\mathbf{1}_N$ is unitarily equivalent to the operator $\mathbf{1}_{M_\rho}\mathrm{Op}(\psi_\rho\otimes\mathbb{1}_n)\mathbf{1}_{N_\rho}$, where the symbol ψ_ρ, given by $\psi_\rho(\xi) := \psi(\rho\xi)$, is supported in a ball of radius 1. For the symbol norm $\mathbf{N}$, defined in Definition 2.8, we have $\mathbf{N}^{(m,m)}(\psi_\rho;1,1) = \mathbf{N}^{(m,m)}(\psi;1,\rho) = \max_{|\alpha|\leqslant m}\sup_{\xi\in\mathbb{R}^d}\rho^{|\alpha|}|\partial_\xi^\alpha\psi(\xi)|$, for every $m\in\mathbb{N}_0$.

For each $a\in\mathbb{Z}^d$, we choose a function $\phi_a\in C_c^\infty(\mathbb{R}^d)$ with $\phi_a|_{Q_a}=1$, supported in the ball $B_{2\sqrt{d}}(a)$ and such that for every multi-index $\alpha\in\mathbb{N}_0^d$ we have

$$\sup_{a\in\mathbb{Z}^d}\sup_{x\in\mathbb{R}^d}|\partial_x^\alpha\phi_a(x)| \leqslant \tilde{C}_{|\alpha|}, \tag{6.179}$$

with constants $\tilde{C}_{|\alpha|}>0$. Suppose now that $Q_a\cap M_\rho\neq\emptyset$ and $\operatorname{dist}(a,N_\rho)\geqslant 3\sqrt{d}$. Then [Sob14, Thm. 3.2] yields the bound

$$\|1_{Q_a\cap M_\rho}\mathrm{Op}(\psi_\rho)1_{N_\rho}\|_1 \leqslant C_1\big(\operatorname{dist}(a,N_\rho)\big)^{-m}\mathbf{N}^{(m+d,m+d)}(\phi_a\psi_\rho;2\sqrt{d},1), \tag{6.180}$$

for arbitrary $m \in \mathbb{N}$, where the constant $C_1 > 0$ is independent of ρ, a, M and N. If instead $\operatorname{dist}(a, N_\rho) < 3\sqrt{d}$, [Sob14, Thm. 3.1] yields the bound

$$\|1_{Q_a \cap M_\rho} \operatorname{Op}(\psi_\rho) 1_{N_\rho}\|_1 \leqslant \| \operatorname{Op}^l(\phi_a \psi_\rho)\|_1 \leqslant C_2 \big(2\sqrt{d}\big)^d \mathbf{N}^{(d+1,d+1)}(\phi_a \psi_\rho; 2\sqrt{d}, 1), \tag{6.181}$$

where the constant $C_2 > 0$ is also independent of ρ, a, M and N. Using the estimate (6.179), we combine (6.180) and (6.181) to obtain the bound

$$\|1_{Q_a \cap M_\rho} \operatorname{Op}(\psi_\rho) 1_{N_\rho}\|_1 \leqslant C'(1 + \operatorname{dist}(a, N_\rho)^2)^{-\frac{m}{2}} \max_{|\alpha| \leqslant n+d} \sup_{\xi \in \mathbb{R}^d} \rho^{|\alpha|} |\partial_\xi^\alpha \psi(\xi)|, \tag{6.182}$$

with constant $C' > 0$ independent of ρ, a, M and N, for arbitrary $m \in \mathbb{N}$ and $a \in \mathbb{Z}^d$. The bound easily extends to the matrix-valued symbol $\psi_\rho \otimes \mathbb{1}_n$. Choosing $m = d + \beta + 1$, we estimate

$$\begin{aligned}
\|\mathbf{1}_M \operatorname{Op}(\psi \otimes \mathbb{1}_n) \mathbf{1}_N\|_1 &\leqslant \sum_{a \in \mathbb{Z}^d} \|\mathbf{1}_{Q_a \cap M_\rho} \operatorname{Op}(\psi_\rho \otimes \mathbb{1}_n) \mathbf{1}_{N_\rho}\|_1 \\
&\leqslant C' \max_{|\alpha| \leqslant 2d+\beta+1} \sup_{\xi \in \mathbb{R}^d} \rho^{|\alpha|} |\partial_\xi^\alpha \psi(\xi)| \sum_{k=0}^\infty \sum_{\substack{a \in \mathbb{Z}^d \colon\, Q_a \cap M_\rho \neq \varnothing \\ k \leqslant \operatorname{dist}(a, N_\rho) \leqslant k+1}} (1 + k^2)^{\frac{-d-\beta-1}{2}} \\
&\leqslant C_\beta C' \max_{|\alpha| \leqslant 2d+\beta+1} \sup_{\xi \in \mathbb{R}^d} \rho^{|\alpha|} |\partial_\xi^\alpha \psi(\xi)| \sum_{k=0}^\infty (1 + (k+1)^2)^{\frac{\beta}{2}} (1 + k^2)^{\frac{-d-\beta-1}{2}} \\
&=: C_\beta C \max_{|\alpha| \leqslant 2d+\beta+1} \sup_{\xi \in \mathbb{R}^d} \rho^{|\alpha|} |\partial_\xi^\alpha \psi(\xi)|.
\end{aligned} \tag{6.183}$$

The constant C is independent of ρ, M and N. □

In Section 6.5 it will often be necessary to obtain bounds for operators with symbol given by a power of ψ and control the dependence on the corresponding exponent. This is the content of the following

Corollary 6.16. *Let $\psi \in \mathbb{C}_c^\infty(\mathbb{R}^d)$ be supported in a ball of radius $b + 1$ centred about the origin and let $p \in \mathbb{N}$. Let $M, N \subseteq \mathbb{R}^d$ be as in Lemma 6.15. Then the operator $M \operatorname{Op}(\psi^p) N$ is trace class and there exists a constant $C > 0$, which is independent of p, M and N, such that*

$$\|\mathbf{1}_M \operatorname{Op}(\psi^p \otimes \mathbb{1}_n) \mathbf{1}_N\|_1 \leqslant C_\beta C p^{2d+\beta+1}. \tag{6.184}$$

Proof. For the function ψ^p, we compute

$$\max_{|\alpha| \leqslant 2d+\beta+1} \sup_{\xi \in \mathbb{R}^d} (b+1)^{|\alpha|} |\partial_\xi^\alpha \psi^p(\xi)| \leqslant C' p^{2d+\beta+1} \tag{6.185}$$

with a constant $C' > 0$ independent of p, M and N. Therefore, the desired bound follows. □

In order to prove an upper bound for the remaining operator, we first need to obtain an estimate for the non-smooth Dirac symbol from the just obtained estimate for smooth symbols. The proof follows the ideas in [Sob14] and overlaps to a large extent with the proof of Lemma 3.9. Therefore, the proof given here is kept a bit shorter. We refer to the proof of Lemma 3.9 for a more detailed version of some of the arguments.

Lemma 6.17. *Let $\psi \in \mathbb{C}_c^\infty(\mathbb{R}^d)$ with $\operatorname{supp}(\psi) \subset B_{b+1}(0)$. Let M, N be as in Lemma 6.15 with arbitrary $\beta \geqslant 0$, C_β independent of L and b, and such that*

$$|\{x \in \mathbb{Z}^d : Q_x \cap M \neq \varnothing\}| \leqslant C_M L^d, \tag{6.186}$$

where Q_x denotes the closed unit cube centred about x and $C_M > 0$ is a constant independent of L and b. Then there exists a constant $C > 0$, which is independent of L, b, M and N, such that for every $L \geqslant \max(b+1, 2)$ we have

$$\left\| \mathbf{1}_M \operatorname{Op}\left(\psi \mathcal{D}\right) \mathbf{1}_N \right\|_1 \leqslant C(C_\beta + C_M) \log L, \tag{6.187}$$

where C_β is the corresponding constant from Lemma 6.15.

Proof. Let $L \geqslant \max(b+1, 2)$. We define the Lipschitz continuous function $\tau : \mathbb{R}^d \to \mathbb{R}_+$ by

$$\tau(\xi) := \frac{1}{4}\sqrt{\frac{1}{L^2} + |\xi|^2}. \tag{6.188}$$

By [Hör03, Thm.1.4.10] we obtain a sequence of centres $(\xi_j)_{j\in\mathbb{N}} \subset \mathbb{R}^d$ such that the balls of radius $\tau_j := \tau(\xi_j)$ about the points ξ_j cover $\mathbb{R}^d$, i.e. $\bigcup_{j\in\mathbb{N}} B_{\tau_j}(\xi_j) = \mathbb{R}^d$ and such that at most $N_0 < \infty$ balls intersect in any given point, where N_0 only depends on the dimension d. Furthermore, there is a partition of unity $(\psi_j)_{j\in\mathbb{N}}$ subordinate to this covering, such that for every multi-index $\alpha \in \mathbb{N}_0^d$ we have

$$\sup_{j\in\mathbb{N}} \sup_{\xi\in\mathbb{R}^d} |\partial_\xi^\alpha \psi_j(\xi)| \leqslant \tilde{C}_{|\alpha|} \tau(\xi)^{-|\alpha|}, \tag{6.189}$$

with constants $\tilde{C}_{|\alpha|} > 0$. By the Lipschitz continuity of τ we obtain the inequality

$$\frac{4}{5}\tau(\xi) \leqslant \tau_j \leqslant \frac{4}{3}\tau(\xi), \qquad \xi \in B_{\tau_j}(\xi_j) \tag{6.190}$$

for every $j \in \mathbb{N}$.

As $\operatorname{supp}(\psi) \subset B_{b+1}(0)$, there is a finite, b-dependent index set $J \subset \mathbb{N}$ with $\bigcup_{j\in J} B_{\tau_j}(\xi_j) \supseteq \operatorname{supp}(\psi\mathcal{D})$. We divide J into the two parts

$$J_1 := \{j \in J : B_{\tau_j}(\xi_j) \cap \{0\} \neq \varnothing\} \qquad \text{and} \qquad J_2 := J \setminus J_1. \tag{6.191}$$

The finite-intersection property implies the upper bound $|J_1| \leqslant N_0$. We estimate

$$\left\| \mathbf{1}_M \operatorname{Op}\left(\psi\mathcal{D}\right)\mathbf{1}_N \right\|_1 \leqslant \sum_{j\in J_1} \left\| \mathbf{1}_M \operatorname{Op}\left(\psi_j\psi\mathcal{D}\right)\mathbf{1}_N \right\|_1 + \sum_{j\in J_2} \left\| \mathbf{1}_M \operatorname{Op}\left(\psi_j\psi\mathcal{D}\right)\mathbf{1}_N \right\|_1. \tag{6.192}$$

If $j \in J_1$, we subdivide the set M along $\mathbb{Z}^d$ and estimate

$$\left\| \mathbf{1}_M \operatorname{Op}\left(\psi_j\psi\mathcal{D}\right)\mathbf{1}_N \right\|_1 \leqslant \sum_{x\in\mathbb{Z}^d:\ Q_x\cap M\neq\varnothing} \left\| \operatorname{Op}^l\left(\phi_x\psi_j \otimes \mathbb{1}_n\right)\right\|_1 \left\| \operatorname{Op}\left(\psi\mathcal{D}\right)\right\|, \tag{6.193}$$

where the functions $\phi_x \in C_c^\infty(\mathbb{R}^d)$ with $\phi_x|_{Q_x} = 1$ are supported in balls $B_{r_1}(x)$ for some radius $r_1 > 0$ and Op^l denotes the standard left-quantisation functor, cf. Section 2.1.4. As we have $\left\| \operatorname{Op}\left(\psi\mathcal{D}\right)\right\| = \|\psi\|_\infty$, it remains to estimate the trace norm of the operator $\operatorname{Op}^l\left(\phi_x\psi_j \otimes \mathbb{1}_n\right)$. Using that $0 \in B_{\tau_j}(\xi_j)$ for all $j \in J_1$, property (6.190) guarantees that $\phi_x\psi_j$ is compactly supported in $B_{r_1}(x) \times B_{\frac{1}{3L}}(\xi_j)$. Therefore, an application of Lemma 3.3 yields

$$\| \operatorname{Op}^l\left(\phi_x\psi_j \otimes \mathbb{1}_n\right)\| \leqslant \frac{C_1}{L^d}, \tag{6.194}$$

where the constant $C_1 > 0$ is independent of L and b. This, in turn, provides, in combination with (6.186), the bound

$$\sum_{j\in J_1} \left\| \mathbf{1}_M \operatorname{Op}\left(\psi_j\psi\mathcal{D}\right)\mathbf{1}_N \right\|_1 \leqslant N_0\, C_1 C_M \|\psi\|_\infty, \tag{6.195}$$

where the right-hand side is independent of L and b.

If instead $j \in J_2$, the symbol $\psi_j\psi\mathcal{D}$ is smooth with $\operatorname{supp}\psi_j\psi\mathcal{D} \subset B_{\tau_j}(\xi_j)$. We apply Lemma 6.15 with $\psi = \psi_j\psi\mathcal{D}$ and obtain

$$\left\|\mathbf{1}_M \operatorname{Op}\left(\psi_j\psi\mathcal{D}\right)\mathbf{1}_N\right\|_1 \leqslant C_\beta C_2 \max_{|\alpha|\leqslant 2d+\beta+1} \sup_{\xi\in\mathbb{R}^d} \tau_j^{|\alpha|}|\partial_\xi^\alpha \psi_j\psi\mathcal{D}(\xi)| \leqslant C_\beta C_3, \tag{6.196}$$

where we used (6.189) as well as (6.190) and the constants $C_2, C_3 > 0$ are independent of $j \in J_2$, as well as of L, b, M and N. Therefore,

$$\sum_{j\in J_2} \left\|\mathbf{1}_M \operatorname{Op}\left(\psi_j\psi\mathcal{D}\right)\mathbf{1}_N\right\|_1 \leqslant C_\beta C_3|J_2| \leqslant C_\beta C_4 \int_{B_{2(b+1)}(0)} \tau(\xi)^{-d}\mathrm{d}\xi, \tag{6.197}$$

where the constant $C_4 > 0$ is independent of L, b, M and N. The last inequality is a consequence of the finite-intersection property and (6.190). We abbreviate $\rho := 2(b+1)$ and write the right-hand side of (6.197) as

$$C_\beta C_4|S^{d-1}| \int_0^{L\rho} \frac{r^{d-1}}{\left(\sqrt{1+r^2}\right)^d}\,\mathrm{d}r \leqslant C_\beta C_5 \log(\rho L), \tag{6.198}$$

for some constant $C_5 > 0$ that is independent of L, b, M and N. This estimate, together with (6.197), (6.195) and (6.192) concludes the proof of the Lemma, as $L \geqslant \max(b+1, 2)$ and C_β is independent of L and b. □

In order to utilise this estimate, we need to further study the remaining operator $\mathbf{1}_{H_{V,L}}X_g$. As in Section 6.3 (cf. (6.82)) we split the set $H_{V,L} = [0, L]^d$ into d parts and rewrite the operator as

$$\mathbf{1}_{H_{V,L}}X_g = \sum_{n=1}^d \mathbf{1}_{H_{L,d,k}} \sum_{\mathcal{M}\subseteq\{1,\ldots,d\}\setminus\{k\}} (-1)^{|\mathcal{M}|}\left[g\left(\mathbf{1}_{H_\mathcal{M}}X\mathbf{1}_{H_\mathcal{M}}\right) - g\left(\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}X\mathbf{1}_{H_{\mathcal{M}\cup\{k\}}}\right)\right], \tag{6.199}$$

where we recall

$$H_{L,d,k} = \{x \in H_{V,L} :\ \forall j \in \{1,\ldots,d\} \setminus \{k\} :\ x_j \leqslant x_k\}. \tag{6.200}$$

We relabel coordinates in suitable way to reduce (6.199) to a sum of expressions of the form

$$\mathbf{1}_{H_{L,d,k}}\Big(g\left(\mathbf{1}_{H_k}X\mathbf{1}_{H_k}\right) - g\left(\mathbf{1}_{H_{k-1}}X\mathbf{1}_{H_{k-1}}\right)\Big), \tag{6.201}$$

with $H_k := \mathbb{R}_+^k \times \mathbb{R}^{d-k}$, for a given $k \in \{1,\ldots,d\}$. The structure of these expressions makes them easier to analyse for monomials and we are now ready to establish the upper bound for the trace norm of the remaining operator (6.175). This is the content of the following

Theorem 6.18. *Let $X = \operatorname{Op}(\psi\mathcal{D})$ and $g : \mathbb{R} \to \mathbb{C}$ be an entire function with $g(0) = 0$. Then there exists a constant $C > 0$, independent of L and b, such that for all $L \geqslant \max(b+1, 2)$ the bound*

$$\Big\|\sum_{V\in\mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}}X_g\Big\|_1 \leqslant C\log L \tag{6.202}$$

holds.

Proof. Let $L \geqslant \max(b+1, 2)$. By suitable rotation and translation, the analysis above and the triangle inequality, it suffices to consider expressions of the form

$$\left\|\mathbf{1}_{H_{L,d,k}}\Big(g\left(\mathbf{1}_{H_k}X\mathbf{1}_{H_k}\right) - g\left(\mathbf{1}_{H_{k-1}}X\mathbf{1}_{H_{k-1}}\right)\Big)\right\|_1. \tag{6.203}$$

We first prove the required bound (6.203) for monomial test function. Writing out the operator in (6.203), we see that every term contains at least one occurrence of the projection $\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k}$, and by Hölder's inequality and the triangle inequality, it suffices to consider trace norms of the form

$$\left\|\mathbf{1}_{H_{L,d,k}}\left(\mathbf{1}_{H_k}X\right)^p\left(\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k}\right)\right\|_1, \tag{6.204}$$

for $p \in \mathbb{N}$. In the case $p = 1$, the desired bound follows immediately from Lemma 6.17. For $p \geqslant 2$, we again introduce several sets "in between" $H_{L,d,k}$ and $H_{k-1} \setminus H_k$. To do so, we first define the sets

$$M_\alpha := \{x \in \mathbb{R}^d : \ \forall j \in \{1, \dots, d\} \setminus \{k\} : \ |x_j| \leqslant \alpha |x_k|\}, \tag{6.205}$$

for real numbers $\alpha > 0$. The required sets are then given by $V_j := H_k \cap [-(j+1)L, (j+1)L]^d \cap M_{j+1}$, for $j \in \{1, \dots, p-1\}$. We set $V_0 := H_{L,d,k}$. Clearly, the sets V_j, $j \in \{0, \dots, p-1\}$, fulfil condition (6.186) with $C_M = p^d$. The sets $M = V_j$, $N = H_k \setminus V_{j+1}$, $j \in \{0, \dots, p-2\}$, and the sets $M = V_{p-1}$, $N = H_{k-1} \setminus H_k$ also fulfil condition (6.177) with $C_\beta = C'_\beta p^d$ and $\beta = d$, where $C'_\beta > 0$ is independent of p, L and b. Therefore, Lemma 6.17, in combination with Hölder's inequality and the triangle inequality, yields

$$\begin{aligned} \big\| \mathbf{1}_{H_{L,d,k}} (\mathbf{1}_{H_k} X)^p (\mathbf{1}_{H_k} - \mathbf{1}_{H_{k-1}}) \big\|_1 &\leqslant \sum_{j=0}^{p-2} \big\| \mathbf{1}_{V_j} X (\mathbf{1}_{H_k} - \mathbf{1}_{V_{j+1}}) \big\|_1 + \big\| \mathbf{1}_{V_{p-1}} X (\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k}) \big\|_1 \\ &\leqslant \sum_{j=0}^{p-1} C_j p^d \log L \leqslant C p^{d+1} \log L, \end{aligned} \tag{6.206}$$

with a constant $C > 0$ independent of L, b and p. This proves the theorem for monomials. The extension to analytic functions works in the usual way, cf., for example, the proof of Lemma 6.13. □

6.4.1. Proof of Theorem 6.1. In order to prove one of the main results of this chapter, Theorem 6.1, it just remains to collect the ingredients from Sections 6.3 and 6.4.

Proof of Theorem 6.1. By assumption the function h is an entire function, with $h(0) = 0$. We set $X := \mathrm{Op}(\psi \mathcal{D})$, where ψ and $\mathcal{D}$ are defined in (6.1). With all the requirements of Theorem 6.8 being fulfilled, the theorem yields

$$\begin{aligned} \operatorname{tr}_{L^2(\mathbb{R}^d) \otimes \mathbb{C}^n} &\Big[h(\mathbf{1}_{\Lambda_L} \mathrm{Op}(\psi \mathcal{D}) \mathbf{1}_{\Lambda_L}) - \sum_{V \in \mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}} \mathrm{Op}(\psi \mathcal{D})_{V,h} \Big] \\ &= \sum_{m=0}^{d-1} (2L)^{d-m} A_{m,h,b} + O(1), \end{aligned} \tag{6.207}$$

as $L \to \infty$. The coefficients $A_{m,h,b}$ are defined in (6.2). Therefore, it remains to consider the trace of the operator

$$\sum_{V \in \mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}} \mathrm{Op}(\psi \mathcal{D})_{V,h}. \tag{6.208}$$

By Theorem 6.18 we have

$$\operatorname{tr}_{L^2(\mathbb{R}^d) \otimes \mathbb{C}^n} \Big[\sum_{V \in \mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}} \mathrm{Op}(\psi \mathcal{D})_{V,h} \Big] \leqslant \Big\| \sum_{V \in \mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}} \mathrm{Op}(\psi \mathcal{D})_{V,h} \Big\|_1 \leqslant C \log L, \tag{6.209}$$

with a constant C independent of L and b. This concludes the proof of the theorem. □

6.5. Commutation in momentum space

With the upper bound being established, the remaining task is to extend the asymptotic expansion to the logarithmic term and to compute the corresponding coefficient. Similarly to the strategy used to obtain an enhanced area law as, for example, shown in Chapter 4, we divide this task into two steps. The first step is to separate the smooth cut-off functions ψ from the projections $\mathrm{Op}(\mathcal{D})$ with discontinuous symbol and commute all occurrences of $\mathrm{Op}(\psi)$ to the right of the operator. The second step is to compute the asymptotic expansion for the resulting operator. This is done in Section 6.6. As stated in the introduction, we are only able to do this last step in the case that the test function is a polynomial of degree three or less. Nonetheless, we are able to do the commutation for arbitrary entire functions g with $g(0) = 0$. As this would be necessary for a potential extension of Theorem 6.3 to entire test functions, we still carry out the proof in this general setting in this section, although Theorem 6.3 only requires the commutation results for polynomial of degree three or less.

The idea for the commutation of the smooth symbols ψ is to mirror the analysis done in the case of an enhanced area law, while treating the projections $\mathrm{Op}(\mathcal{D})$ in the same way as the projections on a basic domain in the enhanced area law case, cf. Section 4.2 for an example of the enhanced area law case. The usual idea is to obtain trace-class bounds for the commutator of $\mathrm{Op}(\psi)$, for $\psi \in \mathbb{C}_c^\infty(\mathbb{R}^d)$, with the projection $\mathbf{1}_{\Omega_L}$ on some scaled subset $\Omega_L \subset \mathbb{R}^d$. But one can only hope to obtain bounds of order L^{d-1} for this commutator, cf. Lemma 3.6. Therefore, we require an extended procedure, which makes use of the structure of the operator $X_{V,g}$, here. Nevertheless, it will be vital to use the estimates established in Section 6.4 for the smooth symbol ψ. We summarise the result of this commutation procedure in the following theorem which we prove at the end of this section, when the necessary intermediate results are established.

Theorem 6.19. *Let $X = \mathrm{Op}(\psi\mathcal{D})$ and $g : \mathbb{R} \to \mathbb{C}$ be an entire function with $g(0) = 0$. Then*

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\sum_{V\in\mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}} X_{V,g} - \sum_{V\in\mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}} \mathrm{Op}\left(\mathcal{D}\right)_{V,g} \mathbf{1}_{H_{V,L}} \mathrm{Op}\left(g(\psi\otimes\mathbb{1}_n)\right)\right] = O(1), \quad (6.210)$$

as $L \to \infty$, where we recall

$$Y_{F,g} = \sum_{k=0}^{d} (-1)^k \sum_{G\in\mathcal{F}_F^{(k)}} g(\mathbf{1}_{H_G} Y \mathbf{1}_{H_G}) \quad (6.211)$$

for $Y \in \{X, \mathrm{Op}(\mathcal{D})\}$.

We begin by establishing the required bounds for polynomial test functions and extend this to entire test functions in Section 6.5.2.

6.5.1. Commutation for monomial test functions. As in (6.201) we reduce the structure of the operator $\mathbf{1}_{H_{V,L}} X_g$ to a sum of expressions of the following form

$$\mathbf{1}_{H_{L,d,k}}\Big(g\big(\mathbf{1}_{H_k} X \mathbf{1}_{H_k}\big) - g\big(\mathbf{1}_{H_{k-1}} X \mathbf{1}_{H_{k-1}}\big)\Big), \quad (6.212)$$

where we recall $H_k = \mathbb{R}_+^k \times \mathbb{R}^{d-k}$, for a given $k \in \{1, \dots, d\}$, as well as

$$H_{L,d,k} = \{x \in H_{V,L} : \forall j \in \{1, \dots, d\} \setminus \{k\} : x_j \leqslant x_k\}. \quad (6.213)$$

We now analyse the difference of the traces of the operator (6.212), with $X = \mathrm{Op}(\psi\mathcal{D})$ and g given by a monomial, and the same operator with all occurrences of $\mathrm{Op}(\psi)$ commuted to the right. More precisely, we want to find a bound for

$$\begin{aligned}\Big|\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[&\mathbf{1}_{H_{V,L}}\Big(\big(\mathbf{1}_{H_k}\mathrm{Op}(\psi\mathcal{D})\mathbf{1}_{H_k}\big)^p - \big(\mathbf{1}_{H_{k-1}}\mathrm{Op}(\psi\mathcal{D})\mathbf{1}_{H_{k-1}}\big)^p\Big)\mathbf{1}_{H_{L,d,k}} \\ &- \mathbf{1}_{H_{V,L}}\Big(\big(\mathbf{1}_{H_k}\mathrm{Op}(\mathcal{D})\mathbf{1}_{H_k}\big)^p - \big(\mathbf{1}_{H_{k-1}}\mathrm{Op}(\mathcal{D})\mathbf{1}_{H_{k-1}}\big)^p\Big)\mathbf{1}_{H_{L,d,k}}\mathrm{Op}(\psi^p\otimes\mathbb{1}_n)\Big]\Big|, \end{aligned} \quad (6.214)$$

for given $k \in \{1, \dots, d\}$ and $p \in \mathbb{N}$. This is the goal of the present section.

The proof of this bound is split into several lemmas contained in this section. As in Section 6.3, we start with Hilbert-Schmidt norm estimates, which present a large part of the technical challenge and then build an estimate for the absolute value of the trace from there. The idea to prove the occurring Hilbert-Schmidt bounds is similar to the one employed in the proof of Lemma 6.11, in the sense that we define a family of sets depending on power functions ϕ_m, $m \in \{1, \dots, p-1\}$, which will allow us to "transport" the decay of the integral kernel along multiple occurrences of the projections $\mathbf{1}_{H_k}$ respectively $\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k}$. Although, in this case we need different sets. To define the relevant sets, we take a closer look at the boundary of H_k. We note that

$$\partial H_k = \{x \in H_k : \min_{1 \leqslant j \leqslant k} x_j = 0\} \tag{6.215}$$

and we have that

$$\operatorname{dist}(x, \partial H_k) \geqslant \min_{1 \leqslant j \leqslant d} |x_j|, \tag{6.216}$$

for all $x \in \mathbb{R}^d$. We now define a family of "thickened up" versions of the boundary of H_k. To do so, let $\phi : [0, \infty[\to [0, \infty[$ be a measurable function. We define

$$\big(\partial H_k\big)_\phi := \{x \in \mathbb{R}^d : \operatorname{dist}(x, \partial H_k) < \phi(\|x\|_\infty)\}, \tag{6.217}$$

where $\|x\|_\infty := \max_{1 \leqslant j \leqslant d} |x_j|$. During the proof of (6.214), it is necessary to split the boundary of H_k into two parts. For real numbers $\alpha > 0$, we recall the definition of the sets

$$M_\alpha = \{x \in \mathbb{R}^d : \ \forall j \in \{1, \dots, d\} \setminus \{k\} : \ |x_j| \leqslant \alpha |x_k|\}, \tag{6.218}$$

and split the set $\big(\partial H_k\big)_\phi$ into the two subsets

$$\big(\partial H_k\big) \cap M_\alpha \quad \text{and} \quad \big(\partial H_k\big) \cap M_\alpha^c. \tag{6.219}$$

Comparing this with H_{k-1}, we see that, for every $\alpha > 0$, we have $\partial_{H_{k-1}} H_k \subset M_\alpha^c$, where $\partial_{H_{k-1}} H_k$ is the boundary of H_k in H_{k-1}. This will be crucial in the proof of Lemma 6.21.

We also need the same objects for the boundary of $H_{k-1} \setminus H_k$. We define

$$\big(\partial(H_{k-1} \setminus H_k)\big)_\phi := \{x \in \mathbb{R}^d : \operatorname{dist}(x, \partial(H_{k-1} \setminus H_k) < \phi(\|x\|_\infty)\} \tag{6.220}$$

and note that $\partial_{H_{k-1}}(H_{k-1} \setminus H_k) = \partial_{H_{k-1}} H_k \subset M_\alpha^c$, for all $\alpha > 0$. With these definitions at hand, we are ready to prove the Hilbert-Schmidt bounds required to commute $\operatorname{Op}(\psi)$ with $\mathbf{1}_{H_k}$ respectively $\mathbf{1}_{H_{k-1} \setminus H_k}$.

Lemma 6.20. *Let $p \in \mathbb{N}$ and $X_1, \dots, X_p$ be bounded translation-invariant integral operators, each satisfying the estimate* (6.45). *Let $k \in \{1, \dots, d\}$ and let $\phi : [0, \infty[\to [0, \infty[$ be given by $\phi(x) := \frac{1}{8}\sqrt{\max(0, x-p)}$. For $m \in \{1, \dots, p\}$, let $V_m \subseteq H_k$ be measurable. Then there exists a constant $C > 0$, independent of all V_m and p, such that, for every measurable $\Omega_1 \subseteq \big(\partial H_k\big)_\phi \cap M_3$, we have*

$$\Big\| \mathbf{1}_{\Omega_1} X_1 \Big(\prod_{m=1}^{p-1} \mathbf{1}_{V_m} X_{m+1} \Big) (\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k}) \Big\|_2 \leqslant C d^{\frac{p}{2}} p^{\frac{d+2}{2}}, \tag{6.221}$$

and for every measurable $\Omega_2 \subseteq \big(\partial(H_{k-1} \setminus H_k)\big)_\phi \cap M_3$, we have

$$\Big\| \mathbf{1}_{\Omega_2} X_1 \Big(\prod_{m=1}^{p-1} (\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k}) X_{m+1} \Big) \mathbf{1}_{V_p} \Big\|_2 \leqslant C d^{\frac{p}{2}} p^{\frac{d+2}{2}}. \tag{6.222}$$

Furthermore, let $\Omega' \subseteq M_1$ be measurable and $P_m \in \{\mathbf{1}_{H_k}, (\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k})\}$, for $m \in \{1, \dots, p-1\}$. Then there exists a constant $C' > 0$, independent of Ω' and p, such that, for every measurable $\Omega_3 \subseteq \big(\partial H_k\big)_\phi \cap M_2^c$, we have

$$\Big\| \mathbf{1}_{\Omega_3} X_1 \Big(\prod_{m=1}^{p-1} P_m X_{m+1} \Big) \mathbf{1}_{\Omega'} \Big\|_2 \leqslant C' d^{\frac{p}{2}} p^{\frac{d+2}{2}}, \tag{6.223}$$

and for every measurable $\Omega_4 \subseteq \big(\partial(H_{k-1} \setminus H_k)\big)_\phi \cap M_2^c$*, we have*

$$\Big\|\mathbf{1}_{\Omega_4} X_1 \Big(\prod_{m=1}^{p-1} P_m X_{m+1}\Big) \mathbf{1}_{\Omega'}\Big\|_2 \leqslant C' d^{\frac{p}{2}} p^{\frac{d+2}{2}}. \tag{6.224}$$

Proof. The proof employs a strategy similar to the one employed in the proof of Lemma 6.11. Therefore, some of the steps are carried out in less detail. We begin with the proof of (6.221) and start with the case $p = 1$. For every $x \in \Omega_1$, we have that $x_k \geqslant 0$, as otherwise we have, using that ϕ is monotone,

$$|x_k| \leqslant \operatorname{dist}(x, \partial H_k) < \phi(\|x\|_\infty) \leqslant \phi(3|x_k|) = \frac{\sqrt{\max(0, 3|x_k| - 1)}}{8}, \tag{6.225}$$

which leads to a contradiction. Therefore, for every $x \in \Omega_1$, we have that $\operatorname{dist}(x, H_{k-1} \setminus H_k) \geqslant x_k$. In particular we have $\operatorname{dist}(\Omega_1, H_{k-1} \setminus H_k) > \frac{1}{3}$, as in the case $x \in \Omega_1$ with $x_k \leqslant \frac{1}{3}$, we would have $\|x\|_\infty \leqslant 1$ and therefore $x \notin \big(\partial H_k\big)_\phi$. We apply Lemma 6.7 with $M = \Omega_1$, $N = H_{k-1} \setminus H_k$ and φ given by $\varphi(x) = x_k$. We recall that $\operatorname{dist}(x, \partial H_k) \geqslant \min_{1\leqslant j\leqslant d} |x_j|$ and compute

$$\begin{aligned}\int_{\Omega_1} \frac{1}{x_k^d}\,\mathrm{d}x &= \sum_{l=1}^{d} \int_{\Omega_1 \cap \{x \in \mathbb{R}^d:\ |x_l| = \min_{1\leqslant j\leqslant d} |x_j|\}} \frac{1}{x_k^d}\,\mathrm{d}x \\ &\leqslant (d-1) \int_{\frac{1}{3}}^{\infty} \frac{2^{d-1}(3x_k)^{d-2}\phi(3x_k)}{x_k^d}\,\mathrm{d}x_k \leqslant \frac{C'}{2\sqrt{3}} \int_{\frac{1}{3}}^{\infty} \frac{x_k^{d-\frac{3}{2}}}{x_k^d}\,\mathrm{d}x_k = C',\end{aligned} \tag{6.226}$$

where we used that $x_k \neq \min_{1\leqslant j\leqslant d} |x_j|$, as otherwise $x_k \leqslant \operatorname{dist}(x, \partial H_k) < \phi(\|x\|_\infty) \leqslant \phi(3x_k)$, which again leads to a contradiction. Therefore, Lemma 6.7 yields the desired constant $C > 0$, such that

$$\big\|\mathbf{1}_{\Omega_1} X_1 (\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k})\big\|_2 \leqslant C. \tag{6.227}$$

This proves (6.221) in the case $p = 1$. We now turn to the case $p \geqslant 2$. For $m \in \{1, \ldots, p-1\}$, we define the sets

$$\Gamma_m := V_m \cap \big(\partial H_k\big)_{\phi_m} \cap M_{\alpha_m}, \tag{6.228}$$

with $\alpha_m := 3 + \frac{m}{p}$ and the functions $\phi_m : [0, \infty[\to [0, \infty[$ given by

$$\phi_m(x) := \tfrac{1}{8}\big(1 + \tfrac{m}{p}\big) \max\big(0, x - p + m\big)^{1 - \frac{1}{2d^m} + \varepsilon}, \tag{6.229}$$

where we set $\varepsilon := \frac{1}{2d^p}$ for the remaining part of the proof. We first consider the Hilbert-Schmidt norm of the operator $\mathbf{1}_{\Omega_1} X_1 \mathbf{1}_{V_1 \setminus \Gamma_1}$. Let $x \in \Omega_1$ and $y \in B_{\frac{\phi_1(\|x\|_\infty)}{4p}}(x)$, then we have

$$\|y\|_\infty > \|x\|_\infty - \tfrac{\phi_1(\|x\|_\infty)}{4p} \geqslant \|x\|_\infty - \tfrac{\|x\|_\infty - p + 1}{16p} = \tfrac{(16p-1)\|x\|_\infty + (p-1)}{16p}, \tag{6.230}$$

where we used that $\|x\|_\infty > p$. A short computation yields

$$\frac{1 + \frac{1}{p}}{8} \frac{16p - 1}{16p} = \frac{16p + 16 - 1 - \frac{1}{p}}{128p} > \frac{1}{8} + \frac{1}{4p} \frac{1 + \frac{1}{p}}{8}. \tag{6.231}$$

With this, the monotonicity of ϕ_1 and its definition, we obtain the bound

$$\begin{aligned}\phi_1(\|y\|_\infty) &\geqslant \phi_1\big(\tfrac{(16p-1)\|x\|_\infty+(p-1)}{16p}\big)\\ &\geqslant \Big(\tfrac{1}{8}+\tfrac{1}{4p}\tfrac{1+1/p}{8}\Big)\tfrac{16p}{16p-1}\max\big(0,\tfrac{(16p-1)\|x\|_\infty+(p-1)}{16p}-(p-1)\big)^{1-\frac{1}{2d}+\varepsilon}\\ &\geqslant \tfrac{1}{8}(\|x\|_\infty-p+1)^{1-\frac{1}{2d}+\varepsilon}+\tfrac{1}{4p}\tfrac{1+1/p}{8}(\|x\|_\infty-p+1)^{1-\frac{1}{2d}+\varepsilon}\\ &> \phi(\|x\|_\infty)+\tfrac{\phi_1(\|x\|_\infty)}{4p}. \end{aligned}\tag{6.232}$$

We conclude

$$\operatorname{dist}(y,\partial H_k)\leqslant \operatorname{dist}(x,\partial H_k)+\tfrac{\phi_1(\|x\|_\infty)}{4p}<\phi(\|x\|_\infty)+\tfrac{\phi_1(\|x\|_\infty)}{4p}<\phi_1(\|y\|_\infty),\tag{6.233}$$

i.e. $y\in\big(\partial H_k\big)_{\phi_1}$. We also have

$$\begin{aligned}\|y\|_\infty &< \|x\|_\infty+\tfrac{\phi_1(\|x\|_\infty)}{4p}\leqslant \tfrac{16p+1}{16p}\|x\|_\infty\leqslant \tfrac{16p+4+1/p}{16p}\|x\|_\infty-(3+\tfrac{1}{p})\tfrac{\phi_1(\|x\|_\infty)}{4p}\\ &\leqslant \tfrac{48p+12+3/p}{16p}|x_k|-(3+\tfrac{1}{p})\tfrac{\phi_1(\|x\|_\infty)}{4p}\leqslant(3+\tfrac{1}{p})\Big(|x_k|-\tfrac{\phi_1(\|x\|_\infty)}{4p}\Big)<(3+\tfrac{1}{p})|y_k|,\end{aligned}\tag{6.234}$$

i.e. $y\in M_{\alpha_1}$. Therefore, for every $x\in\Omega_1$, we have $\operatorname{dist}(x,V_1\setminus\Gamma_1)\geqslant\frac{\phi_1(\|x\|_\infty)}{4p}$. As $\|x\|_\infty>p$, for all $x\in\Omega_1$, we know in particular that $\operatorname{dist}(\Omega_1,V_1\setminus\Gamma_1)>\frac{1}{32p}$. We now apply Lemma 6.7 with $M=\Omega_1$, $N=V_1\setminus\Gamma_1$ and φ given by $\varphi(x)=\frac{\phi_1(\|x\|_\infty)}{4p}$. For the corresponding integral, we compute

$$\begin{aligned}&\int_{\Omega_1}\frac{(4p)^d}{\phi_1(\|x\|_\infty)^d}\,\mathrm{d}x\\ &\quad=\sum_{l=1}^{d}\sum_{\mu\in\{1,\dots,d\}\setminus\{l\}}\int_{\Omega_1\cap\{x\in\mathbb{R}^d:\ |x_l|=\|x\|_\infty\}\cap\{x\in\mathbb{R}^d:\ |x_\mu|=\min_{1\leqslant j\leqslant d}|x_j|\}}\frac{(4p)^d}{\phi_1(\|x\|_\infty)^d}\,\mathrm{d}x\\ &\quad\leqslant d(d-1)(64p)^d\int_p^\infty\frac{x_l^{d-2}\phi(x_l)}{(x_l-p+1)^{d-\frac{1}{2}+d\varepsilon}}\,\mathrm{d}x_l\\ &\quad\leqslant\frac{d(d-1)(64p)^d}{8}\int_1^\infty\frac{(x_l+p-1)^{d-2}\sqrt{x_l}}{x_l^{d-\frac{1}{2}+d\varepsilon}}\,\mathrm{d}x_l\\ &\quad\leqslant\frac{C'p^d}{\varepsilon},\end{aligned}\tag{6.235}$$

with a constant $C'>0$, independent of V_1 and p. Therefore, Lemma 6.7 yields a constant $C_1>0$, independent of V_1 and p, such that

$$\big\|\mathbf{1}_{\Omega_1}X_1\mathbf{1}_{V_1\setminus\Gamma_1}\big\|_2\leqslant C_1\sqrt{\frac{p^d}{\varepsilon}}.\tag{6.236}$$

We continue with the intermediate terms. Let $m\in\{1,\dots,p-2\}$, then we want to find a bound for the Hilbert-Schmidt norm of the operators $\mathbf{1}_{\Gamma_m}X_{m+1}\mathbf{1}_{V_{m+1}\setminus\Gamma_{m+1}}$. Let $x\in\Gamma_m$ and $y\in B_{\frac{\phi_{m+1}(\|x\|_\infty)}{8p}}(x)$, then we have

$$\|y\|_\infty>\|x\|_\infty-\tfrac{\phi_{m+1}(\|x\|_\infty)}{8p}\geqslant\|x\|_\infty-\tfrac{\|x\|_\infty-p+m+1}{32p}=\tfrac{(32p-1)\|x\|_\infty+(p-m-1)}{32p},\tag{6.237}$$

where we used that $\|x\|_\infty>p-m$. A short computation yields

$$\frac{1+\frac{m+1}{p}}{8}\frac{32p-1}{32p}=\frac{32p+32(m+1)-1-\frac{m+1}{p}}{256p}>\frac{1+\frac{m}{p}}{8}+\frac{1}{8p}\frac{1+\frac{m+1}{p}}{8}.\tag{6.238}$$

With this, the monotonicity of ϕ_{m+1} and its definition, we obtain the bound

$$\begin{aligned}\phi_{m+1}(\|y\|_\infty) &\geqslant \phi_{m+1}\big(\tfrac{(32p-1)\|x\|_\infty+(p-m-1)}{32p}\big)\\&\geqslant \Big(\tfrac{1+m/p}{8}+\tfrac{1}{8p}\tfrac{1+(m+1)/p}{8}\Big)\tfrac{32p}{32p-1}\Big(\tfrac{(32p-1)\|x\|_\infty+(p-m-1)}{32p}-(p-m-1)\Big)^{1-\frac{1}{2d^{m+1}}+\varepsilon}\\&\geqslant \tfrac{1+m/p}{8}(\|x\|_\infty-p+m+1)^{1-\frac{1}{2d^{m+1}}+\varepsilon}+\tfrac{1}{8p}\tfrac{1+(m+1)/p}{8}(\|x\|_\infty-p+m+1)^{1-\frac{1}{2d^{m+1}}+\varepsilon}\\&> \phi_m(\|x\|_\infty)+\tfrac{\phi_{m+1}(\|x\|_\infty)}{8p}.\end{aligned}\tag{6.239}$$

We conclude

$$\operatorname{dist}(y,\partial H_k)\leqslant \operatorname{dist}(x,\partial H_k)+\tfrac{\phi_{m+1}(\|x\|_\infty)}{8p}<\phi_m(\|x\|_\infty)+\tfrac{\phi_{m+1}(\|x\|_\infty)}{8p}<\phi_{m+1}(\|y\|_\infty),\tag{6.240}$$

i.e. $y\in\big(\partial H_k\big)_{\phi_{m+1}}$. We also have

$$\begin{aligned}\|y\|_\infty &< \|x\|_\infty+\tfrac{\phi_{m+1}(\|x\|_\infty)}{8p}\leqslant \tfrac{32p+1}{32p}\|x\|_\infty\leqslant \tfrac{32p+4+(m+1)/p}{32p}\|x\|_\infty-(3+\tfrac{m+1}{p})\tfrac{\phi_{m+1}(\|x\|_\infty)}{8p}\\&\leqslant \tfrac{96p+12+3(m+1)/p+32m+4m/p+m(m+1)/p^2}{32p}|x_k|-(3+\tfrac{m+1}{p})\tfrac{\phi_{m+1}(\|x\|_\infty)}{8p}\\&\leqslant (3+\tfrac{m+1}{p})\big(|x_k|-\tfrac{\phi_{m+1}(\|x\|_\infty)}{8p}\big)<(3+\tfrac{m+1}{p})|y_k|,\end{aligned}\tag{6.241}$$

i.e. $y\in M_{\alpha_{m+1}}$. Therefore, for every $x\in\Gamma_m$, we have $\operatorname{dist}(x,V_{m+1}\setminus\Gamma_{m+1})\geqslant\frac{\phi_{m+1}(\|x\|_\infty)}{8p}$. As $\|x\|_\infty>p-m$, for all $x\in\Gamma_m$, we know in particular that $\operatorname{dist}(\Gamma_m,V_{m+1}\setminus\Gamma_{m+1})>\frac{1}{64p}$. We again apply Lemma 6.7. Now with $M=\Gamma_m$, $N=V_{m+1}\setminus\Gamma_{m+1}$ and φ given by $\varphi(x)=\frac{\phi_{m+1}(\|x\|_\infty)}{8p}$. For the corresponding integral, we compute

$$\begin{aligned}&\int_{\Gamma_m}\frac{(8p)^d}{\phi_{m+1}(\|x\|_\infty)^d}\,\mathrm{d}x\\&\leqslant\sum_{l=1}^{d}\sum_{\mu\in\{1,\dots,d\}\setminus\{l\}}\int_{\left(\partial H_k\right)_{\phi_m}\cap\{x\in\mathbb{R}^d:\ |x_l|=\|x\|_\infty\}\cap\{x\in\mathbb{R}^d:\ |x_\mu|=\min_{1\leqslant j\leqslant d}|x_j|\}}\frac{(8p)^d}{\phi_{m+1}(\|x\|_\infty)^d}\,\mathrm{d}x\\&\leqslant d(d-1)(128p)^d\int_{p-m}^{\infty}\frac{(x_l)^{d-2}\phi_m(x_l)}{(x_l-p+m+1)^{d-\frac{1}{2d^m}+d\varepsilon}}\,\mathrm{d}x_l\\&\leqslant\frac{d(d-1)(128p)^d}{4}\int_1^\infty\frac{(x_l+p-m-1)^{d-2}x_l^{1-\frac{1}{2d^m}+\varepsilon}}{x_l^{d-\frac{1}{2d^m}+d\varepsilon}}\,\mathrm{d}x_l\\&\leqslant\frac{C'p^d}{\varepsilon},\end{aligned}\tag{6.242}$$

with a constant $C'>0$, independent of V_m, V_{m+1} and p. Therefore, Lemma 6.7 yields a constant $C_{m+1}>0$, independent of V_m, V_{m+1} and p, such that

$$\left\|\mathbf{1}_{\Gamma_m}X_{m+1}\mathbf{1}_{V_{m+1}\setminus\Gamma_{m+1}}\right\|_2\leqslant C_{m+1}\sqrt{\frac{p^d}{\varepsilon}}.\tag{6.243}$$

It remains to estimate the last operator $\mathbf{1}_{\Gamma_{p-1}}X_p(\mathbf{1}_{H_{k-1}}-\mathbf{1}_{H_k})$. For every $x\in\Gamma_{p-1}$, we have that $x_k\geqslant 0$, as $\Gamma_{p-1}\subset H_k$. Therefore, we have, for every $x\in\Gamma_{p-1}$, that $\operatorname{dist}(x,H_{k-1}\setminus H_k)\geqslant x_k$. In particular we have $\operatorname{dist}(\Gamma_{p-1},H_{k-1}\setminus H_k)>\frac14$, as in the case $x\in\Gamma_{p-1}$ with $x_k\leqslant\frac14$, we would have

$\|x\|_\infty \leqslant 1$ and therefore $x \notin \left(\partial H_k\right)_{\phi_{p-1}}$. We apply Lemma 6.7 with $M = \Gamma_{p-1}$, $N = H_{k-1} \setminus H_k$ and φ given by $\varphi(x) = x_k$. We recall that $\operatorname{dist}(x, \partial H_k) \geqslant \min_{1 \leqslant j \leqslant d} |x_j|$ and compute

$$
\begin{aligned}
\int_{\Gamma_{p-1}} \frac{1}{x_k^d}\,\mathrm{d}x &= \sum_{l=1}^{d} \int_{\left(\partial H_k\right)_{\phi_{p-1}} \cap M_4 \cap \{x \in \mathbb{R}^d:\ |x_l| = \min_{1 \leqslant j \leqslant d} |x_j|\}} \frac{1}{x_k^d}\,\mathrm{d}x \\
&\leqslant (d-1) \int_{\frac{1}{4}}^{\infty} \frac{2^d (4x_k)^{d-2} \phi_{p-1}(4x_k)}{x_k^d}\,\mathrm{d}x_k \\
&\leqslant 8^d (d-1) \int_{\frac{1}{4}}^{\infty} x_k^{-1-\frac{1}{2d^{p-1}}+\varepsilon}\,\mathrm{d}x_k \leqslant C' \frac{1}{\varepsilon},
\end{aligned} \tag{6.244}
$$

where the constant $C' > 0$ is independent of V_{p-1} and p. Therefore, Lemma 6.7 yields a constant $C_p > 0$, independent of V_{p-1} and p, such that

$$
\left\|\mathbf{1}_{\Gamma_{p-1}} X_p (\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k})\right\|_2 \leqslant C_p \sqrt{\frac{1}{\varepsilon}}. \tag{6.245}
$$

Repeated use of the triangle inequality, followed by Hölder's inequality, yields

$$
\begin{aligned}
&\left\|\mathbf{1}_{\Omega_1} X_1 \Big(\prod_{m=1}^{p-1} \mathbf{1}_{V_m} X_{m+1}\Big)(\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k})\right\|_2 \\
&\leqslant \sum_{m=0}^{p-2} \left\|\mathbf{1}_{\Omega_1} X_1 \Big(\prod_{j=1}^{m} \mathbf{1}_{\Gamma_j} X_{j+1}\Big) \mathbf{1}_{V_{m+1} \setminus \Gamma_{m+1}} X_{m+2} \Big(\prod_{j=m+2}^{p-1} \mathbf{1}_{V_j} X_{j+1}\Big)(\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k})\right\|_2 \\
&\qquad + \left\|\mathbf{1}_{\Omega_1} X_1 \Big(\prod_{j=1}^{p-1} \mathbf{1}_{\Gamma_j} X_{j+1}\Big)(\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k})\right\|_2 \\
&\leqslant \left\|\mathbf{1}_{\Omega_1} X_1 \mathbf{1}_{V_1 \setminus \Gamma_1}\right\|_2 + \sum_{m=1}^{p-2} \left\|\mathbf{1}_{\Gamma_m} X_{m+1} \mathbf{1}_{V_{m+1} \setminus \Gamma_{m+1}}\right\|_2 + \left\|\mathbf{1}_{\Gamma_{p-1}} X_p (\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k})\right\|_2 \\
&\leqslant C d^{\frac{p}{2}} p^{\frac{d+2}{2}},
\end{aligned} \tag{6.246}
$$

where we combined estimates (6.236), (6.243) and (6.245) and used the definition of ε in the last line. The constant C is independent of p and V_m, for every $m \in \{1, \dots, p-1\}$. This proves (6.221) for $p \geqslant 2$.

The bound (6.222) reduces to (6.221) through the reflection $S : \mathbb{R}^d \to \mathbb{R}^d$ along the hyperplane orthogonal to the kth coordinate, as we have $S(H_k) = H_{k-1} \setminus H_k$ and $S(M_\alpha) = M_\alpha$, for every $\alpha > 0$.

We continue with the proof of (6.223). We again begin with the case $p = 1$. Let $x \in \Omega_3 \subset (M_2)^c$ and $y \in B_{\frac{\|x\|_\infty}{4}}(x)$. Then we have

$$
\|y\|_\infty > \tfrac{3}{4}\|x\|_\infty = \tfrac{1}{2}\|x\|_\infty + \tfrac{\|x\|_\infty}{4} > |x_k| + \tfrac{\|x\|_\infty}{4} > |y_k|, \tag{6.247}
$$

i.e. $y \notin M_1$. Therefore, we have $\operatorname{dist}(x, \Omega') \geqslant \operatorname{dist}(x, M_1) \geqslant \frac{\|x\|_\infty}{4}$. In particular we have $\operatorname{dist}(\Omega_3, \Omega') > \frac{1}{4}$. We apply Lemma 6.7 with $M = \Omega_3$, $N = \Omega'$ and φ given by $\varphi(x) = \frac{\|x\|_\infty}{4}$. We recall that $\operatorname{dist}(x, \partial H_k) \geqslant \min_{1\leqslant j\leqslant d} |x_j|$ and compute

$$\int_{\Omega_3} \frac{4^d}{\|x\|_\infty^d}\,\mathrm{d}x = \sum_{l=1}^{d} \sum_{\mu\in\{1,\dots,d\}\setminus\{l\}} \int_{\Omega_3\cap\{x\in\mathbb{R}^d:\ |x_l|=\|x\|_\infty\}\cap\{x\in\mathbb{R}^d:\ |x_\mu|=\min_{1\leqslant j\leqslant d}|x_j|\}} \frac{4^d}{\|x\|_\infty^d}\,\mathrm{d}x$$
$$\leqslant d(d-1)\int_1^\infty \frac{4^d 2^d x_l^{d-2}\phi(x_l)}{x_l^d}\,\mathrm{d}x_l \leqslant \frac{C}{2}\int_1^\infty \frac{x_l^{d-\frac{3}{2}}}{x_l^d}\,\mathrm{d}x_l = C, \quad (6.248)$$

with a constant $C > 0$, independent of Ω'. Therefore, Lemma 6.7 yields the desired constant $C' > 0$, independent of Ω', such that

$$\left\|\mathbf{1}_{\Omega_3} X_1 \mathbf{1}_{\Omega'}\right\|_2 \leqslant C'. \quad (6.249)$$

This proves (6.223) in the case $p = 1$. We now turn to the case $p \geqslant 2$. For $m \in \{1,\dots,p-1\}$, let $V_m \in \{H_k, H_{k-1}\setminus H_k\}$ be the set corresponding to the projection P_m. For $m \in \{1,\dots,p-1\}$, we define the sets

$$\Gamma_m := V_m \cap \left(\partial H_k\right)_{\phi_m} \cap M_{\alpha_m}^c, \quad (6.250)$$

with $\alpha_m := 2 - \frac{m}{2p}$ and $\phi_m : [0,\infty[\to [0,\infty[$ given by

$$\phi_m(x) = \tfrac{1}{8}\left(1+\tfrac{m}{p}\right)\max\left(0, x-p+m\right)^{1-\frac{1}{2d^m}+\varepsilon}, \quad (6.251)$$

as in the proof of (6.221). We recall $\varepsilon = \frac{1}{2d^p}$. Again, we begin with the Hilbert-Schmidt norm of the operator $\mathbf{1}_{\Omega_3} X_1 \mathbf{1}_{V_1\setminus\Gamma_1}$. Let $x \in \Omega_3$ and $y \in B_{\frac{\phi_1(\|x\|_\infty)}{4p}}(x)$, then we have, as in the proof of (6.221), that $y \in \left(\partial H_k\right)_{\phi_1}$. It remains to check that also $y \in M_{\alpha_1}^c$. We estimate

$$\begin{aligned}\|y\|_\infty &> \|x\|_\infty - \tfrac{\phi_1(\|x\|_\infty)}{4p} \geqslant \tfrac{(16p-1)\|x\|_\infty}{16p} \geqslant \tfrac{16p-3+1/(2p)}{16p}\|x\|_\infty + \left(2-\tfrac{1}{2p}\right)\tfrac{\phi_1(\|x\|_\infty)}{4p}\\ &\geqslant \tfrac{32p-6+1/p}{16p}|x_k| + \left(2-\tfrac{1}{2p}\right)\tfrac{\phi_1(\|x\|_\infty)}{4p} \geqslant \left(2-\tfrac{1}{2p}\right)\left(|x_k| + \tfrac{\phi_1(\|x\|_\infty)}{4p}\right) \geqslant \left(2-\tfrac{1}{2p}\right)|y_k|, \quad (6.252)\end{aligned}$$

where we used that $\|x\|_\infty > p$. Therefore, for every $x \in \Omega_3$, we have $\operatorname{dist}(x, V_1\setminus\Gamma_1) \geqslant \frac{\phi_1(\|x\|_\infty)}{4p}$. As $\|x\|_\infty > p$, for all $x \in \Omega_3$, we know in particular that $\operatorname{dist}(\Omega_3, V_1\setminus\Gamma_1) > \frac{1}{32p}$. We now apply Lemma 6.7 with $M = \Omega_3$, $N = V_1\setminus\Gamma_1$ and φ given by $\varphi(x) = \frac{\phi_1(\|x\|_\infty)}{4p}$. For the corresponding integral we compute, in the same way as in (6.235), that

$$\int_{\Omega_3} \frac{(4p)^d}{\phi_1(\|x\|_\infty)^d}\,\mathrm{d}x$$
$$= \sum_{l=1}^{d} \sum_{\mu\in\{1,\dots,d\}\setminus\{l\}} \int_{\Omega_3\cap\{x\in\mathbb{R}^d:\ |x_l|=\|x\|_\infty\}\cap\{x\in\mathbb{R}^d:\ |x_\mu|=\min_{1\leqslant j\leqslant d}|x_j|\}} \frac{(4p)^d}{\phi_1(\|x\|_\infty)^d}\,\mathrm{d}x \leqslant \frac{Cp^d}{\varepsilon}, \quad (6.253)$$

with a constant $C > 0$, independent of V_1 and p. Therefore, Lemma 6.7 yields a constant $C_1' > 0$, independent of V_1 and p, such that

$$\left\|\mathbf{1}_{\Omega_3} X_1 \mathbf{1}_{V_1\setminus\Gamma_1}\right\|_2 \leqslant C_1'\sqrt{\frac{p^d}{\varepsilon}}. \quad (6.254)$$

We continue with the intermediate terms. Let $m \in \{1,\dots,p-2\}$, then we want to find a bound for the Hilbert-Schmidt norm of the operators $\mathbf{1}_{\Gamma_m} X_{m+1} \mathbf{1}_{V_{m+1}\setminus\Gamma_{m+1}}$. Let $x \in \Gamma_m$ and $y \in B_{\frac{\phi_{m+1}(\|x\|_\infty)}{8p}}(x)$, then we have, as in the proof of (6.221), that $y \in \big(\partial H_k\big)_{\phi_{m+1}}$. It remains to check that also $y \in M^c_{\alpha_{m+1}}$. We estimate

$$\begin{aligned}\|y\|_\infty &> \|x\|_\infty - \tfrac{\phi_{m+1}(\|x\|_\infty)}{8p} \geqslant \tfrac{(32p-1)\|x\|_\infty}{32p} \geqslant \tfrac{32p-3+(m+1)/(2p)}{32p}\|x\|_\infty + \big(2-\tfrac{m+1}{2p}\big)\tfrac{\phi_{m+1}(\|x\|_\infty)}{8p} \\ &\geqslant \tfrac{64p-16m-6}{32p}|x_k| + \big(2-\tfrac{m+1}{2p}\big)\tfrac{\phi_{m+1}(\|x\|_\infty)}{8p} \geqslant \big(2-\tfrac{m+1}{2p}\big)\big(|x_k| + \tfrac{\phi_{m+1}(\|x\|_\infty)}{8p}\big) \geqslant \big(2-\tfrac{m+1}{2p}\big)|y_k|, \quad (6.255)\end{aligned}$$

where we used that $\|x\|_\infty > p-m$. Therefore, for every $x \in \Gamma_m$, we have $\operatorname{dist}(x, V_{m+1}\setminus\Gamma_{m+1}) \geqslant \frac{\phi_{m+1}(\|x\|_\infty)}{8p}$. As $\|x\|_\infty > p-m$, for all $x \in \Gamma_m$, we know in particular that $\operatorname{dist}(\Gamma_m, V_{m+1}\setminus\Gamma_{m+1}) > \frac{1}{64p}$. We again apply Lemma 6.7. Now with $M = \Gamma_m$, $N = V_{m+1}\setminus\Gamma_{m+1}$ and φ given by $\varphi(x) = \frac{\phi_{m+1}(\|x\|_\infty)}{8p}$. We treat the corresponding integral as in (6.242) and obtain

$$\int_{\Gamma_m} \frac{(8p)^d}{\phi_{m+1}(\|x\|_\infty)^d}\,\mathrm{d}x \leqslant \frac{Cp^d}{\varepsilon}, \tag{6.256}$$

with a constant $C > 0$, independent of V_m, V_{m+1} and p. Therefore, Lemma 6.7 yields a constant $C'_{m+1} > 0$, independent of V_m, V_{m+1} and p, such that

$$\big\|\mathbf{1}_{\Gamma_m} X_{m+1}\mathbf{1}_{V_{m+1}\setminus\Gamma_{m+1}}\big\|_2 \leqslant C'_{m+1}\sqrt{\frac{p^d}{\varepsilon}}. \tag{6.257}$$

It remains to estimate the last operator $\mathbf{1}_{\Gamma_{p-1}} X_p \mathbf{1}_{\Omega'}$. Let $x \in \Gamma_{p-1} \subset \big(M_{3/2}\big)^c$ and $y \in B_{\frac{\|x\|_\infty}{6}}(x)$. Then we have

$$\|y\|_\infty > \tfrac{5}{6}\|x\|_\infty = \tfrac{4}{6}\|x\|_\infty + \tfrac{\|x\|_\infty}{6} > |x_k| + \tfrac{\|x\|_\infty}{6} > |y_k|, \tag{6.258}$$

i.e. $y \notin M_1$. Therefore, we have $\operatorname{dist}(x,\Omega') \geqslant \operatorname{dist}(x, M_1) \geqslant \frac{\|x\|_\infty}{6}$. In particular we have $\operatorname{dist}(\Gamma_{p-1},\Omega') > \frac{1}{6}$. We apply Lemma 6.7 with $M = \Gamma_{p-1}$, $N = \Omega'$ and φ given by $\varphi(x) = \frac{\|x\|_\infty}{6}$. We recall that $\operatorname{dist}(x,\partial H_k) \geqslant \min_{1\leqslant j\leqslant d}|x_j|$ and compute

$$\begin{aligned}\int_{\Gamma_{p-1}} \frac{6^d}{\|x\|_\infty^d}\,\mathrm{d}x &= \sum_{l=1}^d \sum_{\mu\in\{1,\dots,d\}\setminus\{l\}} \int_{\Gamma_{p-1}\cap\{x\in\mathbb{R}^d:\ |x_l|=\|x\|_\infty\}\cap\{x\in\mathbb{R}^d:\ |x_\mu|=\min_{1\leqslant j\leqslant d}|x_j|\}} \frac{6^d}{\|x\|_\infty^d}\,\mathrm{d}x \\ &\leqslant d(d-1)\int_1^\infty \frac{12^d x_l^{d-2}\phi_{p-1}(x_l)}{x_l^d}\,\mathrm{d}x_l \leqslant d(d-1)12^d\int_1^\infty x_l^{-1-\frac{1}{2d^{p-1}}+\varepsilon}\,\mathrm{d}x_l \leqslant C\frac{1}{\varepsilon}, \quad (6.259)\end{aligned}$$

with a constant $C > 0$, independent of V_{p-1}, Ω' and p. Therefore, Lemma 6.7 yields a constant $C'_p > 0$, independent of V_{p-1}, Ω' and p, such that

$$\big\|\mathbf{1}_{\Gamma_{p-1}} X_p(\mathbf{1}_{H_{k-1}} - \mathbf{1}_{\Omega'})\big\|_2 \leqslant C'_p\sqrt{\frac{1}{\varepsilon}}. \tag{6.260}$$

As in the proof of (6.221), we combine the estimates (6.254), (6.257) and (6.260) and use the definition of ε to obtain the bound (6.223). This proves (6.223) for $p \geqslant 2$.

As in the proof of the bound (6.222), the bound (6.224) reduces to (6.223) through the reflection along the hyperplane orthogonal to the kth coordinate. This finishes the proof of the lemma. □

Now we combine the trace-class bound from Lemma 6.16 with the Hilbert-Schmidt bounds we just obtained and make use of the structure of the operator in question in order to commute the first $p-1$ occurrences of $\operatorname{Op}(\psi)$ to the right.

Lemma 6.21. *Let $L \geqslant 1$ and $p \in \mathbb{N}$. Then there exists a constant $C > 0$, independent of L and p, such that*

$$\Big| \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \Big[\mathbf{1}_{H_{L,d,k}} \Big(\big(\mathbf{1}_{H_k} \operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_k}\big)^p - \big(\mathbf{1}_{H_{k-1}} \operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_{k-1}}\big)^p - \big(\mathbf{1}_{H_k} \operatorname{Op}(\mathcal{D})\mathbf{1}_{H_k}\big)^{p-1} \operatorname{Op}(\psi^p\mathcal{D})\mathbf{1}_{H_k} + \big(\mathbf{1}_{H_{k-1}} \operatorname{Op}(\mathcal{D})\mathbf{1}_{H_{k-1}}\big)^{p-1} \operatorname{Op}(\psi^p\mathcal{D})\mathbf{1}_{H_{k-1}} \Big) \Big] \Big| \leqslant C(2\sqrt{d})^{p-1}(p-1)^{5d+1}. \tag{6.261}$$

Proof. For $p = 1$, there is nothing to show. Similarly as in the proof of Lemma 6.12, we write

$$\mathbf{1}_{H_{L,d,k}} \Big(\big(\mathbf{1}_{H_{k-1}} \operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_{k-1}}\big)^p - \big(\mathbf{1}_{H_k} \operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_k}\big)^p \Big) \mathbf{1}_{H_{L,d,k}} = \sum_{\pi=(\pi_1,\dots,\pi_{p-1})\in\{0,1\}^{p-1},\pi\neq 0} \mathbf{1}_{H_{L,d,k}} \Big(\prod_{j=1}^{p-1} \operatorname{Op}(\psi\mathcal{D}) P_{\pi(j)} \Big) \operatorname{Op}(\psi\mathcal{D}) \mathbf{1}_{H_{L,d,k}}, \tag{6.262}$$

with $P_0 = \mathbf{1}_{H_k}$ and $P_1 = \mathbf{1}_{H_{k-1}\setminus H_k}$. For the remaining part of the proof, we will only consider one of these terms for a given $\pi \in \{0,1\}^{p-1}$ with $\pi \neq 0$. The estimates for the sum follow by the triangle inequality. The fact that $\pi \neq 0$ guarantees that there is at least one occurrence of the projection $\mathbf{1}_{H_{k-1}\setminus H_k}$. For the given π, we define $p_{1,\pi} := \min\{j \in \{1,\dots,p-1\} : \pi(j) = 1\}$ and $p_{2,\pi} := \max\{j \in \{1,\dots,p-1\} : \pi(j) = 1\}$. The first step is to commute the first occurrence of ψ to the right, i.e. we want to estimate

$$\Big| \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \Big[\mathbf{1}_{H_{L,d,k}} \Big(\operatorname{Op}(\psi\mathcal{D}) P_{\pi(1)} - \operatorname{Op}(\mathcal{D}) P_{\pi(1)} \operatorname{Op}(\psi) \Big) \Big(\prod_{j=2}^{p-1} \operatorname{Op}(\psi\mathcal{D}) P_{\pi(j)} \Big) \operatorname{Op}(\psi\mathcal{D}) \Big] \Big|. \tag{6.263}$$

We write

$$\begin{aligned} \operatorname{Op}(\psi\mathcal{D}) P_{\pi(1)} &- \operatorname{Op}(\mathcal{D}) P_{\pi(1)} \operatorname{Op}(\psi) \\ &= \operatorname{Op}(\mathcal{D}) \big[(\mathbf{1} - P_{\pi(1)} + P_{\pi(1)}) \operatorname{Op}(\psi) P_{\pi(1)} - P_{\pi(1)} \operatorname{Op}(\psi) (\mathbf{1} - P_{\pi(1)} + P_{\pi(1)}) \big] \\ &= \operatorname{Op}(\mathcal{D}) \big[(\mathbf{1} - P_{\pi(1)}) \operatorname{Op}(\psi) P_{\pi(1)} - P_{\pi(1)} \operatorname{Op}(\psi) (\mathbf{1} - P_{\pi(1)}) \big], \end{aligned} \tag{6.264}$$

where $\mathbf{1} := \mathbf{1}_{\mathbb{R}^d}$ is the corresponding multiplication operator on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$. With this at hand, we bound (6.263) from above by

$$\Big| \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \Big[\mathbf{1}_{H_{L,d,k}} \operatorname{Op}(\mathcal{D}) (\mathbf{1} - P_{\pi(1)}) \operatorname{Op}(\psi) P_{\pi(1)} \Big(\prod_{j=2}^{p-1} \operatorname{Op}(\psi\mathcal{D}) P_{\pi(j)} \Big) \operatorname{Op}(\psi\mathcal{D}) \Big] \Big| + \Big| \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \Big[\mathbf{1}_{H_{L,d,k}} \operatorname{Op}(\mathcal{D}) P_{\pi(1)} \operatorname{Op}(\psi) (\mathbf{1} - P_{\pi(1)}) \Big(\prod_{j=2}^{p-1} \operatorname{Op}(\psi\mathcal{D}) P_{\pi(j)} \Big) \operatorname{Op}(\psi\mathcal{D}) \Big] \Big|. \tag{6.265}$$

We will continue to estimate the first trace in (6.265). The second trace works in the same way. To do so, we choose the measurable function $\phi : [0,\infty[\longrightarrow [0,\infty[$ with $\phi(x) := \frac{1}{8}\sqrt{\max(0, x-p)}$ and define the projections $P_{0,\phi} := \mathbf{1}_{(\partial H_k)_\phi \cap H_k}$ and $P_{1,\phi} := \mathbf{1}_{(\partial(H_{k-1}\setminus H_k))_\phi \cap (H_{k-1}\setminus H_k)}$. Then Corollary 6.16 with $\beta = 2d$ and $C_\beta = C'_\beta p^d$, with $C'_\beta > 0$ independent of p, yields that

$$\|(\mathbf{1} - P_{\pi(1)}) \operatorname{Op}(\psi) (P_{\pi(1)} - P_{\pi(1),\phi})\|_1 \leqslant C_0 p^d \tag{6.266}$$

with the constant $C_0 > 0$ being independent of L and p. This allows us to replace the projection $P_{\pi(1)}$ on the right-hand side of $\operatorname{Op}(\psi)$ in the first line of (6.265) with the projection $P_{\pi(1),\phi}$ up to an error term of constant order. As explained earlier in this section, we split the sets $(\partial H_k)_\phi$ and

$\big(\partial(H_{k-1}\setminus H_k)\big)_\phi$ into two subsets, which are disjoint up to sets of measure zero. We choose the parameter $\alpha = \frac{5}{2}$ and define the corresponding projections

$$P^{(1)}_{\pi(1),\phi} := P_{\pi(1),\phi}\mathbf{1}_{M_{5/2}} \qquad \text{and} \qquad P^{(2)}_{\pi(1),\phi} := P_{\pi(1),\phi}\mathbf{1}_{(M_{5/2})^c}. \tag{6.267}$$

We also define the projections

$$\begin{aligned} P^{(3)}_{0,\phi} &:= \mathbf{1}_{(\partial H_k)_\phi}\mathbf{1}_{(H_k)^c}\mathbf{1}_{M_3}, & P^{(4)}_{0,\phi} &:= \mathbf{1}_{(\partial H_k)_\phi}\mathbf{1}_{(H_k)^c}\mathbf{1}_{(M_2)^c},\\ P^{(3)}_{1,\phi} &:= \mathbf{1}_{(\partial(H_{k-1}\setminus H_k))_\phi}\mathbf{1}_{(H_{k-1}\setminus H_k)^c}\mathbf{1}_{M_3}, & P^{(4)}_{1,\phi} &:= \mathbf{1}_{(\partial(H_{k-1}\setminus H_k))_\phi}\mathbf{1}_{(H_{k-1}\setminus H_k)^c}\mathbf{1}_{(M_2)^c} \end{aligned} \tag{6.268}$$

and claim that the trace norms of the operators

$$\begin{aligned} &\big(\mathbf{1}_{(H_k)^c} - P^{(3)}_{0,\phi}\big)\operatorname{Op}(\psi)P^{(1)}_{0,\phi}, && \big(\mathbf{1}_{(H_k)^c} - P^{(4)}_{0,\phi}\big)\operatorname{Op}(\psi)P^{(2)}_{0,\phi},\\ &\big(\mathbf{1}_{(H_{k-1}\setminus H_k)^c} - P^{(3)}_{1,\phi}\big)\operatorname{Op}(\psi)P^{(1)}_{0,\phi}, && \big(\mathbf{1}_{(H_{k-1}\setminus H_k)^c} - P^{(4)}_{1,\phi}\big)\operatorname{Op}(\psi)P^{(2)}_{1,\phi}, \end{aligned} \tag{6.269}$$

are bounded by a constant times p^d, which is independent of L and p. We will only check this for the first operator, the other cases work in the same way. In order to apply Corollary 6.16, we need to check the condition (6.177) for the sets $M = (H_k)^c \setminus \big((\partial H_k)_\phi \cap (H_k)^c \cap M_3\big)$ and $N = M_{5/2} \cap (\partial H_k)_\phi \cap H_k$. We only do so in the case $\rho = 1$, as another choice of ρ would only yield an additional dependence on $\rho = b + 1$ in the constant C_β but we are not concerned with the dependence on b in the present lemma. Let $x \in (H_k)^c \setminus \big((\partial H_k)_\phi \cap (H_k)^c \cap M_3\big)$, then we consider two cases. In the first case we have $x \in (H_k)^c$ and $x \notin (\partial H_k)_\phi$ and therefore

$$\operatorname{dist}(x, M_{5/2} \cap (\partial H_k)_\phi \cap H_k) \geqslant \operatorname{dist}(x, H_k) = \operatorname{dist}(x, \partial H_k) \geqslant \phi(\|x\|_\infty) = \frac{\sqrt{\max(0, \|x\|_\infty - p)}}{8}. \tag{6.270}$$

In the second case we have $x \notin M_3$. Suppose now that $y \in B_{\frac{\|x\|_\infty}{21}}(x)$, then we have

$$\|y\|_\infty > \tfrac{20}{21}\|x\|_\infty = \tfrac{5}{6}\|x\|_\infty + \tfrac{5}{2}\tfrac{\|x\|_\infty}{21} > \tfrac{5}{2}\big(|x_k| + \tfrac{\|x\|_\infty}{21}\big) > \tfrac{5}{2}|y_k|, \tag{6.271}$$

i.e. $y \notin M_{5/2}$. Therefore, in this case we have

$$\operatorname{dist}(x, M_{5/2} \cap (\partial H_k)_\phi \cap H_k) \geqslant \operatorname{dist}(x, M_{5/2}) \geqslant \tfrac{\|x\|_\infty}{21}. \tag{6.272}$$

Combining (6.270) and (6.272), we find a constant $C'_\beta > 0$, independent of L and p, such that the first operator in (6.269) satisfies the requirements of Corollary 6.16 with $\beta = 2d$ and $C_\beta = C'_\beta p^d$. Checking this for the remaining operators in (6.269), Corollary 6.16 yields that the trace norms of the operators in (6.269) are indeed bounded by a constant times p^d independent of L and p. With this at hand, we estimate the first trace in (6.265) by

$$\sum_{l=1}^{2}\Big|\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{H_{L,d,k}}\operatorname{Op}(\mathcal{D})P^{(l+2)}_{\pi(1),\phi}\operatorname{Op}(\psi)P^{(l)}_{\pi(1),\phi}\Big(\prod_{j=2}^{p-1}\operatorname{Op}(\psi\mathcal{D})P_{\pi(j)}\Big)\operatorname{Op}(\psi\mathcal{D})\Big]\Big| + C'_0 p^d. \tag{6.273}$$

with C'_0, independent of L and p.

We now estimate the individual terms in (6.273) by using the cyclic property of the trace to rewrite them as products of Hilbert-Schmidt norms and then applying Lemma 6.20. Here, we have to distinguish between several different cases. In order to apply Lemma 6.20, we note that we have $(\partial H_k)_\phi \subset (\partial H_k)_{\phi_m}$ and $\big(\partial(H_{k-1}\setminus H_k)\big)_\phi \subset \big(\partial(H_{k-1}\setminus H_k)\big)_{\phi_m}$ for all $m \in \{1, \dots, p-1\}$, where $\phi_m : [0,\infty[\to [0,\infty[$ with $\phi_m(x) := \frac{1}{8}\sqrt{\max(0, x-m)}$. We also recall the definitions $p_{1,\pi} = \min\{j \in \{1,\dots,p-1\} : \pi(j) = 1\}$ and $p_{2,\pi} = \max\{j \in \{1,\dots,p-1\} : \pi(j) = 1\}$.

(i) If $l = 1$ and $\pi(1) = 0$, we estimate the corresponding term in (6.273) by

$$\Big\| P_{\pi(p_{2,\pi})} \Big(\prod_{j=p_{2,\pi}+1}^{p-1} \mathrm{Op}(\psi\mathcal{D}) P_{\pi(j)} \Big) \mathrm{Op}(\psi\mathcal{D}) \mathbf{1}_{H_{L,d,k}} \mathrm{Op}(\mathcal{D}) P^{(3)}_{0,\phi} \Big\|_2$$
$$\times \quad \Big\| P^{(1)}_{0,\phi} \Big(\prod_{j=2}^{p_{1,\pi}-1} \mathrm{Op}(\psi\mathcal{D}) P_{\pi(j)} \Big) \mathrm{Op}(\psi\mathcal{D}) P_{\pi(p_{1,\pi})} \Big\|_2 \tag{6.274}$$

and apply (6.221) to obtain the bound

$$C_1 d^{\frac{p-1}{2}} (p-1)^{d+2}, \tag{6.275}$$

where the constant $C_1 > 0$ is independent of L and p.

(ii) If $l = 2$ and $\pi(1) = 0$, we estimate the corresponding term in (6.273) by

$$\big\| \mathbf{1}_{H_{L,d,k}} \mathrm{Op}(\mathcal{D}) P^{(4)}_{0,\phi} \big\|_2 \quad \times \quad \Big\| P^{(2)}_{0,\phi} \Big(\prod_{j=2}^{p-1} \mathrm{Op}(\psi\mathcal{D}) P_{\pi(j)} \Big) \mathrm{Op}(\psi\mathcal{D}) \mathbf{1}_{H_{L,d,k}} \Big\|_2 \tag{6.276}$$

and apply (6.223) to obtain the same bound as in (i).

(iii) If $l = 1$ and $\pi(1) = 1$, we estimate the corresponding term in (6.273) by

$$\big\| \mathbf{1}_{H_{L,d,k}} \mathrm{Op}(\mathcal{D}) P^{(3)}_{1,\phi} \big\|_2 \quad \times \quad \Big\| P^{(1)}_{1,\phi} \Big(\prod_{j=2}^{p_{1,\pi,0}-1} \mathrm{Op}(\psi\mathcal{D}) P_{\pi(j)} \Big) \mathrm{Op}(\psi\mathcal{D}) P_{\pi(p_{1,\pi,0})} \Big\|_2, \tag{6.277}$$

where $p_{1,\pi,0}$ is the smallest $j \in \{2,\dots,p-1\}$ with $\pi(p_{1,\pi,0}) = 0$, in the case that it exists. Otherwise we set $p_{1,\pi,0} = p$ and $P_{p_{1,\pi,0}} = \mathbf{1}_{H_{L,d,k}}$. Then we apply (6.222) to obtain the same bound as in (i).

(iv) If $l = 2$ and $\pi(1) = 1$, we estimate the corresponding term in (6.273) by

$$\big\| \mathbf{1}_{H_{L,d,k}} \mathrm{Op}(\mathcal{D}) P^{(4)}_{1,\phi} \big\|_2 \quad \times \quad \Big\| P^{(2)}_{1,\phi} \Big(\prod_{j=2}^{p-1} \mathrm{Op}(\psi\mathcal{D}) P_{\pi(j)} \Big) \mathrm{Op}(\psi\mathcal{D}) \mathbf{1}_{H_{L,d,k}} \Big\|_2 \tag{6.278}$$

and apply (6.224) to obtain the same bound as in (i).

As we obtain the same bound in all of the cases, we see that (6.273), and with it (6.263), are bounded from above by

$$C_1' d^{\frac{p-1}{2}} (p-1)^{d+2}, \tag{6.279}$$

with $C_1' > 0$ independent of L and p.

We continue by iterating this procedure in order to also commute the following $p-2$ occurrences of $\mathrm{Op}(\psi^m)$, for $m \in \{2,\dots,p-1\}$, to the right. To do so, we need to find an upper bound for

$$\Big| \mathrm{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \Big[\mathbf{1}_{H_{L,d,k}} \Big(\prod_{j=1}^{m-1} \mathrm{Op}(\mathcal{D}) P_{\pi(j)} \Big) X_m \Big(\prod_{j=m+1}^{p-1} \mathrm{Op}(\psi\mathcal{D}) P_{\pi(j)} \Big) \mathrm{Op}(\psi\mathcal{D}) \Big] \Big|, \tag{6.280}$$

where the operator difference X_m is given by

$$\begin{aligned} X_m :&= \mathrm{Op}(\psi^m\mathcal{D}) P_{\pi(m)} - \mathrm{Op}(\mathcal{D}) P_{\pi(m)} \mathrm{Op}(\psi^m) \\ &= \mathrm{Op}(\mathcal{D}) \big[(\mathbf{1} - P_{\pi(m)}) \mathrm{Op}(\psi^m) P_{\pi(m)} - P_{\pi(m)} \mathrm{Op}(\psi^m) (\mathbf{1} - P_{\pi(m)}) \big]. \end{aligned} \tag{6.281}$$

By the triangle inequality it suffices to study the first of these terms. Using the same projections $P^{(j)}_{\pi(m),\phi}$, $j \in \{1,2,3,4\}$, as for the commutation of the first occurrence of ψ, we see that this study reduces to estimating the traces

$$\Big|\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{H_{L,d,k}}\Big(\prod_{j=1}^{m-1}\operatorname{Op}(\mathcal{D})P_{\pi(j)}\Big)X_{m,l}\Big(\prod_{j=m+1}^{p-1}\operatorname{Op}(\psi\mathcal{D})P_{\pi(j)}\Big)\operatorname{Op}(\psi\mathcal{D})\Big]\Big|, \tag{6.282}$$

for the operators $X_{m,l} := \operatorname{Op}(\mathcal{D})P^{(l+2)}_{\pi(m),\phi}\operatorname{Op}(\psi^m)P^{(l)}_{\pi(m),\phi}$, where $l \in \{0,1\}$. As we now applied Corollary 6.16 to the function ψ^m, instead of ψ, we obtain an error term of order $p^d m^{2d+\beta+1}$ which is at most of order $(p-1)^{5d+1}$, due to the required choice of $\beta = 2d$ and $C_\beta = C'_\beta p^d$ in the application of Corollary 6.16. The estimate for (6.282) is obtained, in the same way as the estimate for (6.273), by considering four different cases depending on $l \in \{0,1\}$ and $\pi(m)$ which all reduce to an application of Lemma 6.20.

Therefore, we obtain the bound

$$\Big|\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{H_{L,d,k}}\Big(\prod_{j=1}^{p-1}\operatorname{Op}(\mathcal{D})P_{\pi(j)}\Big)\operatorname{Op}(\psi^p\mathcal{D})\Big]\Big| \leqslant Cd^{\frac{p-1}{2}}(p-1)^{5d+1}, \tag{6.283}$$

with a constant $C > 0$, independent of L and p. Summing up the contributions of all $\pi \in \{0,1\}^{p-1}$ with $\pi \neq 0$, we obtain a constant $C > 0$, independent of L and p, such that

$$\begin{aligned}\Big|\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{H_{L,d,k}}\Big(&(\mathbf{1}_{H_k}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_k})^p - (\mathbf{1}_{H_{k-1}}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{H_{k-1}})^p \\ &- (\mathbf{1}_{H_k}\operatorname{Op}(\mathcal{D})\mathbf{1}_{H_k})^{p-1}\operatorname{Op}(\psi^p\mathcal{D})\mathbf{1}_{H_k} \\ &+ (\mathbf{1}_{H_{k-1}}\operatorname{Op}(\mathcal{D})\mathbf{1}_{H_{k-1}})^{p-1}\operatorname{Op}(\psi^p\mathcal{D})\mathbf{1}_{H_{k-1}}\Big)\Big]\Big| \leqslant C(2\sqrt{d})^{p-1}(p-1)^{5d+1}.\end{aligned} \tag{6.284}$$

This concludes the proof of the lemma. □

In order to find an upper bound for (6.214), it remains to commute $\operatorname{Op}(\psi^p)$ with the projection onto the set $H_{L,d,k}$. To do so, we will first split the set $H_{L,d,k} = \bigcup_{x_k\in[0,L]}[0,x_k]^{k-1}\times\{x_k\}\times[0,x_k]^{d-k}$ into the two disjoint parts

$$H_{L,d,k} = \{x \in H_{L,d,k} : x_k \leqslant \tfrac{L}{2}\} \cup \{x \in H_{L,d,k} : x_k > \tfrac{L}{2}\} =: H^{(1)}_{L,d,k} \cup H^{(2)}_{L,d,k}. \tag{6.285}$$

We note that the set $H^{(2)}_{L,d,k}$ has a measure of order L^d and a distance of order L to the set $H_{k-1}\setminus H_k$. Therefore, we later deal with it using Lemma 6.9. For the set $H^{(1)}_{L,d,k}$, we define, given a measurable function $\phi : [0,\infty[\,\to[0,\infty[$, a "thickened up" version of the boundary of its infinite version, i.e. of the set $H_{\infty,d,k}$, by

$$\begin{aligned}\big(\partial H_{\infty,d,k}\big)_\phi := &\bigcup_{x_k\in[0,\infty[}\,]-\phi(x_k),x_k+\phi(x_k)[^{k-1}\times\{x_k\}\times\,]-\phi(x_k),x_k+\phi(x_k)[^{d-k} \\ &\setminus\bigcup_{x_k\in[0,\infty[}\,]\phi(x_k),x_k-\phi(x_k)[^{k-1}\times\{x_k\}\times\,]\phi(x_k),x_k-\phi(x_k)[^{d-k}.\end{aligned} \tag{6.286}$$

We define the part of this "thickened up" boundary associated to $H^{(1)}_{L,d,k}$ by

$$\big(\partial H_{L,d,k}\big)_\phi := \big\{x \in \big(\partial H_{\infty,d,k}\big)_\phi :\ x_k \in [0,\tfrac{L}{2}]\big\}. \tag{6.287}$$

Next, we provide an estimate for a Hilbert-Schmidt norm involving this set.

Lemma 6.22. *Let $p \in \mathbb{N}$ and $X_1, \dots, X_p$ be bounded translation-invariant integral operators, each satisfying the estimate* (6.45). *Let $k \in \{1, \dots, d\}$. Further let $\phi : [0, \infty[\to [0, \infty[$ be given by $\phi(x) := \frac{1}{p^2}\sqrt{\max(0, px - p)}$. Then, for every measurable $\Omega \subseteq \left(\partial H_{\infty,d,k}\right)_\phi$, there exists a constant $C > 0$, independent of Ω and p, such that*

$$\Big\| \mathbf{1}_\Omega X_1 \Big(\prod_{m=1}^{p-1} \mathbf{1}_{H_k} X_{m+1} \Big) (\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k}) \Big\|_2 \leqslant C d^{\frac{p}{2}} p^{\frac{3d+2}{2}}. \tag{6.288}$$

Proof. The proof is similar to the one of Lemma 6.20. As usual we start with the case $p = 1$. For every $x \in \Omega$, we clearly have $x_k \geqslant 0$ and therefore $\operatorname{dist}(x, H_{k-1} \setminus H_k) \geqslant x_k$. In particular we have $\operatorname{dist}(\Omega, H_{k-1} \setminus H_k) > 1$, as in the case $x \in \Omega$ with $x_k \leqslant 1$, we would have $x \notin \left(\partial H_{\infty,d,k}\right)_\phi$. We apply Lemma 6.7 with $M = \Omega$, $N = H_{k-1} \setminus H_k$ and φ given by $\varphi(x) = x_k$. We note that we have $\phi(x_k) \leqslant \sqrt{x_k}$ and compute

$$\int_\Omega \frac{1}{x_k^d} \, \mathrm{d}x \leqslant C_0 \int_1^\infty \frac{x_k^{d-2} \phi(x_k)}{x_k^d} \, \mathrm{d}x_k = C_0', \tag{6.289}$$

where the constants C_0, C_0' are independent of Ω. Therefore, Lemma 6.7 yields a constant $C > 0$, independent of Ω, such that

$$\big\| \mathbf{1}_\Omega X_1 (\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k}) \big\|_2 \leqslant C. \tag{6.290}$$

This proves the lemma in the case $p = 1$. We now turn to the case $p \geqslant 2$. For $m \in \{1, \dots, p-1\}$, we define the sets

$$\Gamma_m := H_k \cap \left(\partial H_{\infty,d,k}\right)_{\phi_m}, \tag{6.291}$$

with ϕ_m given by

$$\phi_m(x) := \frac{m+1}{p^2} \max\left(0, px - p + m\right)^{1 - \frac{1}{2d^m} + \varepsilon}, \tag{6.292}$$

where we set $\varepsilon := \frac{1}{2d^p}$ for the remaining part of the proof. We first consider the Hilbert-Schmidt norm of the operator $\mathbf{1}_\Omega X_1 \mathbf{1}_{H_k \setminus \Gamma_1}$. Let $x \in \Omega$ and $y \in B_{\frac{\phi_1(x_k)}{2p}}(x)$, then we have

$$y_k > x_k - \tfrac{\phi_1(x_k)}{2p} \geqslant x_k - \tfrac{px_k - p + 1}{2p^2} = \tfrac{(2p^2 - p)x_k + (p-1)}{2p^2}, \tag{6.293}$$

where we used that $x_k > 1$. A short computation yields

$$\tfrac{2}{p^2} \tfrac{2p^2 - p}{2p^2} = \tfrac{4p^2 - 2p}{2p^4} > \tfrac{1}{p^2} + \tfrac{2}{2p^3}. \tag{6.294}$$

With this, the monotonicity of ϕ_1 and its definition, we obtain the bound

$$\begin{aligned} \phi_1(y_k) &\geqslant \phi_1\big(\tfrac{(2p^2-p)x_k + (p-1)}{2p^2}\big) \geqslant \big(\tfrac{1}{p^2} + \tfrac{2}{2p^3}\big) \tfrac{2p^2}{2p^2 - p} \max\left(0, \tfrac{(2p^2-p)x_k + (p-1)}{2p} - (p-1)\right)^{1 - \frac{1}{2d} + \varepsilon} \\ &\geqslant \tfrac{1}{p^2} (px_k - p + 1)^{1 - \frac{1}{2d} + \varepsilon} + \tfrac{2}{2p^3} (px_k - p + 1)^{1 - \frac{1}{2d} + \varepsilon} \geqslant \phi(x_k) + \tfrac{\phi_1(x_k)}{2p}. \end{aligned} \tag{6.295}$$

We conclude

$$\operatorname{dist}(y, \partial H_{\infty,d,k}) \leqslant \operatorname{dist}(x, \partial H_{\infty,d,k}) + \tfrac{\phi_1(x_k)}{2p} < \phi(x_k) + \tfrac{\phi_1(x_k)}{2p} < \phi_1(y_k), \tag{6.296}$$

i.e. $y \in \left(\partial H_{\infty,d,k}\right)_{\phi_1}$. Therefore, for every $x \in \Omega$, we have $\operatorname{dist}(x, H_k \setminus \Gamma_1) \geqslant \frac{\phi_1(x_k)}{2p}$. As $x_k > 1$ for all $x \in \Omega$, we know in particular that $\operatorname{dist}(\Omega, H_k \setminus \Gamma_1) > \frac{1}{p^3}$. We now apply Lemma 6.7 with

$M = \Omega$, $N = H_k \setminus \Gamma_1$ and φ given by $\varphi(x) = \frac{\phi_1(x_k)}{2p}$. Again we have $\phi(x_k) \leqslant \sqrt{x_k}$ and we estimate the corresponding integral by

$$\int_\Omega \frac{(2p)^d}{\phi_1(x_k)^d}\,\mathrm{d}x \leqslant C'p^d \int_1^\infty \frac{x_k^{d-2}\phi(x_k)}{\phi_1(x_k)^d}\,\mathrm{d}x_k \leqslant C'p^{3d}\int_1^\infty x_k^{d-\frac{3}{2}-d+\frac{1}{2}-d\varepsilon}\,\mathrm{d}x_k \leqslant C''\frac{p^{3d}}{\varepsilon}, \quad (6.297)$$

with constants $C', C'' > 0$, independent of Ω and p. Therefore, Lemma 6.7 yields a constant $C_1 > 0$, independent of Ω and p, such that

$$\left\|\mathbf{1}_\Omega X_1 \mathbf{1}_{H_k\setminus\Gamma_1}\right\|_2 \leqslant C_1\sqrt{\frac{p^{3d}}{\varepsilon}}. \quad (6.298)$$

We continue with the intermediate terms. Let $m \in \{1, \dots, p-2\}$, then we want to find a bound for the Hilbert-Schmidt norm of the operators $\mathbf{1}_{\Gamma_m} X_{m+1}\mathbf{1}_{H_k\setminus\Gamma_{m+1}}$. Let $x \in \Gamma_m$ and $y \in B_{\frac{\phi_{m+1}(x_k)}{2p}}(x)$, then we have

$$y_k > x_k - \tfrac{\phi_{m+1}(x_k)}{2p} \geqslant x_k - \tfrac{px_k-p+m+1}{2p^2} = \tfrac{(2p^2-p)x_k+(p-m-1)}{2p^2}, \quad (6.299)$$

where we used that $x_k > \frac{p-m}{p}$. A short computation yields

$$\tfrac{m+2}{p^2}\tfrac{2p^2-p}{2p^2} = \tfrac{2(m+2)p^2-(m+2)p}{2p^4} > \tfrac{2(m+1)p^2+(m+2)p}{2p^4} = \tfrac{m+1}{p^2} + \tfrac{m+2}{2p^3}. \quad (6.300)$$

With this, the monotonicity of ϕ_{m+1} and its definition, we obtain the bound

$$\begin{aligned}\phi_{m+1}(y_k) &\geqslant \phi_{m+1}\big(\tfrac{(2p^2-p)x_k+(p-m-1)}{2p^2}\big)\\ &\geqslant \Big(\tfrac{m+1}{p^2}+\tfrac{m+2}{2p^3}\Big)\tfrac{2p^2}{2p^2-p}\max\big(0, \tfrac{(2p^2-p)x_k+(p-m-1)}{2p} - (p-m-1)\big)^{1-\frac{1}{2d^{m+1}}+\varepsilon}\\ &\geqslant \tfrac{m+1}{p^2}(px_k-p+m+1)^{1-\frac{1}{2d^{m+1}}+\varepsilon} + \tfrac{m+2}{2p^3}(px_k-p+m+1)^{1-\frac{1}{2d^{m+1}}+\varepsilon}\\ &> \phi_m(x_k) + \tfrac{\phi_{m+1}(x_k)}{2p}. \end{aligned} \quad (6.301)$$

We conclude

$$\operatorname{dist}(y, \partial H_{\infty,d,k}) \leqslant \operatorname{dist}(x, \partial H_{\infty,d,k}) + \tfrac{\phi_{m+1}(x_k)}{2p} < \phi_m(x_k) + \tfrac{\phi_{m+1}(x_k)}{2p} < \phi_{m+1}(y_k), \quad (6.302)$$

i.e. $y \in \big(\partial H_{\infty,d,k}\big)_{\phi_{m+1}}$. Therefore, for every $x \in \Gamma_m$, we have $\operatorname{dist}(x, H_k \setminus \Gamma_{m+1}) \geqslant \frac{\phi_{m+1}(x_k)}{2p}$. As $x_k > \frac{p-m}{p}$, for all $x \in \Gamma_m$, we know in particular that $\operatorname{dist}(\Gamma_m, H_k\setminus\Gamma_{m+1}) > \frac{1}{p^3}$. We again apply Lemma 6.7. Now with $M = \Gamma_m$, $N = H_k \setminus \Gamma_{m+1}$ and φ given by $\varphi(x) = \frac{\phi_{m+1}(x_k)}{2p}$. We estimate the corresponding integral

$$\begin{aligned}\int_{\Gamma_m} \frac{(2p)^d}{\phi_{m+1}(x_k)^d}\,\mathrm{d}x \leqslant C'p^d\int_{\frac{p-m}{p}}^\infty \frac{x_k^{d-2}\phi_m(x_k)}{\phi_{m+1}(x_k)^d}\,\mathrm{d}x_k \leqslant C'p^{3d}\int_{\frac{p-m}{p}}^\infty x_k^{d-1-\frac{1}{2d^m}+\varepsilon-d+\frac{1}{2d^m}-d\varepsilon}\,\mathrm{d}x_k&\\ \leqslant C''\frac{p^{3d}}{\varepsilon},&\end{aligned} \quad (6.303)$$

with constants $C', C'' > 0$, independent of Ω and p. Therefore, Lemma 6.7 yields a constant $C_{m+1} > 0$, independent of Ω and p, such that

$$\left\|\mathbf{1}_{\Gamma_m} X_{m+1}\mathbf{1}_{V_{m+1}\setminus\Gamma_{m+1}}\right\|_2 \leqslant C_{m+1}\sqrt{\frac{p^{3d}}{\varepsilon}}. \quad (6.304)$$

It remains to estimate the last operator $\mathbf{1}_{\Gamma_{p-1}} X_p(\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k})$.

For every $x \in \Gamma_{p-1}$, we have $x_k \geqslant 0$ and therefore $\operatorname{dist}(x, H_{k-1} \setminus H_k) \geqslant x_k$. In particular we have $\operatorname{dist}(\Gamma_{p-1}, H_{k-1} \setminus H_k) > \frac{1}{p}$, as in the case $x \in \Gamma_{p-1}$ with $x_k \leqslant \frac{1}{p}$, we would have $x \notin \left(\partial H_{\infty,d,k}\right)_{\phi_{p-1}}$. We apply Lemma 6.7 with $M = \Gamma_{p-1}$, $N = H_{k-1} \setminus H_k$ and φ given by $\varphi(x) = x_k$. We compute

$$\int_{\Gamma_{p-1}} \frac{1}{x_k^d} \, \mathrm{d}x \leqslant C' \int_{\frac{1}{p}}^{\infty} \frac{x_k^{d-2} \phi_{p-1}(x_k)}{x_k^d} \, \mathrm{d}x_k \leqslant C'' \frac{1}{\varepsilon}, \tag{6.305}$$

with constants $C', C'' > 0$, independent of Ω and p. Therefore, Lemma 6.7 yields a constant $C_p > 0$, independent of Ω and p, such that

$$\left\| \mathbf{1}_{\Gamma_{p-1}} X_p (\mathbf{1}_{H_{k-1}} - \mathbf{1}_{H_k}) \right\|_2 \leqslant C_p \sqrt{\frac{1}{\varepsilon}}. \tag{6.306}$$

As in (6.246), we combine the estimates (6.298), (6.304) and (6.306) and use the definition of ε to obtain the bound (6.288). This proves the lemma for $p \geqslant 2$. □

In a similar way as in Lemma 6.21, we now use the derived Hilbert-Schmidt bound to also commute the last occurrence of $\operatorname{Op}(\psi^p)$ to the right.

Lemma 6.23. *Let $L \geqslant 1$ and $p \in \mathbb{N}$. Then there exists a constant $C > 0$, independent of L and p, such that*

$$\begin{aligned} \Big| \operatorname{tr}_{L^2(\mathbb{R}^d) \otimes \mathbb{C}^n} \Big[& \mathbf{1}_{H_{V,L}} \Big(\big(\mathbf{1}_{H_k} \operatorname{Op}(\psi \mathcal{D}) \mathbf{1}_{H_k}\big)^p - \big(\mathbf{1}_{H_{k-1}} \operatorname{Op}(\psi \mathcal{D}) \mathbf{1}_{H_{k-1}}\big)^p \Big) \mathbf{1}_{H_{L,d,k}} \\ & - \mathbf{1}_{H_{V,L}} \Big(\big(\mathbf{1}_{H_k} \operatorname{Op}(\mathcal{D}) \mathbf{1}_{H_k}\big)^p - \big(\mathbf{1}_{H_{k-1}} \operatorname{Op}(\mathcal{D}) \mathbf{1}_{H_{k-1}}\big)^p \Big) \mathbf{1}_{H_{L,d,k}} \operatorname{Op}(\psi^p \otimes \mathbb{1}_n) \Big] \Big| \\ & \leqslant C (2\sqrt{d})^{p-1} p^{7d+1}. \end{aligned} \tag{6.307}$$

Proof. For $p = 1$, there is nothing to show. After an application of Lemma 6.21 it only remains to commute the remaining occurrence of $\operatorname{Op}(\psi^d)$ with $\mathbf{1}_{H_{L,d,k}}$, i.e. we want to find a bound for

$$\begin{aligned} \Big| \operatorname{tr}_{L^2(\mathbb{R}^d) \otimes \mathbb{C}^n} \Big[& \Big(\big(\mathbf{1}_{H_k} \operatorname{Op}(\mathcal{D}) \mathbf{1}_{H_k}\big)^{p-1} \operatorname{Op}(\psi^p \mathcal{D}) - \big(\mathbf{1}_{H_{k-1}} \operatorname{Op}(\mathcal{D}) \mathbf{1}_{H_{k-1}}\big)^{p-1} \operatorname{Op}(\psi^p \mathcal{D}) \Big) \mathbf{1}_{H_{L,d,k}} \\ & - \mathbf{1}_{H_{V,L}} \Big(\big(\mathbf{1}_{H_k} \operatorname{Op}(\mathcal{D}) \mathbf{1}_{H_k}\big)^p - \big(\mathbf{1}_{H_{k-1}} \operatorname{Op}(\mathcal{D}) \mathbf{1}_{H_{k-1}}\big)^p \Big) \mathbf{1}_{H_{L,d,k}} \operatorname{Op}(\psi^p \otimes \mathbb{1}_n) \Big] \Big|. \end{aligned} \tag{6.308}$$

As in the proof of Lemma 6.21 we write

$$\begin{aligned} & \mathbf{1}_{H_{V,L}} \Big(\big(\mathbf{1}_{H_{k-1}} \operatorname{Op}(\mathcal{D}) \mathbf{1}_{H_{k-1}}\big)^{p-1} - \big(\mathbf{1}_{H_k} \operatorname{Op}(\mathcal{D}) \mathbf{1}_{H_k}\big)^{p-1} \Big) \operatorname{Op}(\psi^p \mathcal{D}) \mathbf{1}_{H_{L,d,k}} \\ & \qquad = \sum_{\pi = (\pi_1, \dots, \pi_{p-1}) \in \{0,1\}^{p-1}, \pi \neq 0} \mathbf{1}_{H_{V,L}} \Big(\prod_{j=1}^{p-1} \operatorname{Op}(\mathcal{D}) P_{\pi(j)} \Big) \operatorname{Op}(\psi^p \mathcal{D}) \mathbf{1}_{H_{L,d,k}}, \end{aligned} \tag{6.309}$$

with $P_0 = \mathbf{1}_{H_k}$ and $P_1 = \mathbf{1}_{H_{k-1} \setminus H_k}$. For the remaining part of the proof, we will only consider one of these terms for a given $\pi \in \{0,1\}^{p-1}$ with $\pi \neq 0$. The estimates for the sum follow by the triangle inequality. The fact that $\pi \neq 0$ guarantees that there is at least one occurrence of the projection $\mathbf{1}_{H_{k-1} \setminus H_k}$. For the given π, we define $p_{1,\pi} := \min\{j \in \{1, \dots, p-1\} : \pi(j) = 1\}$ and $p_{2,\pi} := \max\{j \in \{1, \dots, p-1\} : \pi(j) = 1\}$. In order to commute the operator $\operatorname{Op}(\psi^d)$ to the right for the given π we need to estimate

$$\Big| \operatorname{tr}_{L^2(\mathbb{R}^d) \otimes \mathbb{C}^n} \Big[\mathbf{1}_{H_{V,L}} \Big(\prod_{j=1}^{p-1} \operatorname{Op}(\mathcal{D}) P_{\pi(j)} \Big) \operatorname{Op}(\mathcal{D}) \Big(\operatorname{Op}(\psi^p \otimes \mathbb{1}_n) \mathbf{1}_{H_{L,d,k}} - \mathbf{1}_{H_{L,d,k}} \operatorname{Op}(\psi^p \otimes \mathbb{1}_n) \Big) \Big] \Big|. \tag{6.310}$$

We write

$$\begin{aligned}&\operatorname{Op}(\psi^p\mathcal{D})\mathbf{1}_{H_{L,d,k}}-\operatorname{Op}(\mathcal{D})\mathbf{1}_{H_{L,d,k}}\operatorname{Op}(\psi^p\otimes\mathbb{1}_n)\\&\quad=\operatorname{Op}(\mathcal{D})\big[(\mathbf{1}-\mathbf{1}_{H_{L,d,k}})\operatorname{Op}(\psi^p\otimes\mathbb{1}_n)\mathbf{1}_{H_{L,d,k}}-\mathbf{1}_{H_{L,d,k}}\operatorname{Op}(\psi^p\otimes\mathbb{1}_n)(\mathbf{1}-\mathbf{1}_{H_{L,d,k}})\big].\end{aligned}\tag{6.311}$$

By the triangle inequality it suffices to only study one of these terms, as the other one works in an analogous way. Therefore, we continue by a finding a bound for

$$\Big|\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{H_{V,L}}\Big(\prod_{j=1}^{p-1}\operatorname{Op}(\mathcal{D})P_{\pi(j)}\Big)\operatorname{Op}(\mathcal{D})(\mathbf{1}-\mathbf{1}_{H_{L,d,k}})\operatorname{Op}(\psi^p\otimes\mathbb{1}_n)\mathbf{1}_{H_{L,d,k}}\Big]\Big|.\tag{6.312}$$

We now replace the projections $\mathbf{1}_{H_{L,d,k}}$ and $(\mathbf{1}-\mathbf{1}_{H_{L,d,k}})$ by projections which correspond to "thickened up" versions of $\partial H_{L,d,k}$ with the help of Corollary 6.16. To do so, let $\phi:=\phi_p:[0,\infty[\,\to[0,\infty[$ be given by $\phi(x):=\phi_p(x):=\frac{1}{p^2}\sqrt{\max(0,px-p)}$. We define the projections

$$P_\phi^{(1)}:=\mathbf{1}_{H_{L,d,k}}-\mathbf{1}_{\{x\in H_{L,d,k}:\ x\in(\partial H_{L,d,k})_\phi\text{ or }L/2<x_k\}}\tag{6.313}$$

and

$$P_\phi^{(2)}:=\mathbf{1}_{(H_{L,d,k})^c}-\mathbf{1}_{\{x\in(H_{L,d,k})^c:\ x\in(\partial H_{L,d,k})_\phi\text{ or }L/2<x_k<2L\}}.\tag{6.314}$$

Then Corollary 6.16 yields a constant C_1, independent of L and p, such that

$$\begin{aligned}&\|(\mathbf{1}-\mathbf{1}_{H_{L,d,k}})\operatorname{Op}(\psi^p\otimes\mathbb{1}_n)P_\phi^{(1)}\|_1\leqslant C_1p^{7d+1},\\&\|P_\phi^{(2)}\operatorname{Op}(\psi^p\otimes\mathbb{1}_n)(\mathbf{1}_{H_{L,d,k}}-P_\phi^{(1)})\|_1\leqslant C_1p^{7d+1}.\end{aligned}\tag{6.315}$$

We will only check this for the first trace norm. The second one works in a similar way. As in the proof of Lemma 6.21, we only verify the condition (6.177) in the case $\rho=1$. Let $x\in H_{L,d,k}\setminus\big(\partial H_{L,d,k}\big)_\phi$ such that $x_k\leqslant\frac{L}{2}$. Then we have

$$\operatorname{dist}(x,(H_{L,d,k})^c)=\operatorname{dist}(x,\partial H_{L,d,k})\geqslant\phi(x_k)=\tfrac{1}{p^2}\sqrt{\max(0,px_k-p)}.\tag{6.316}$$

Suppose now that $r>0$ and that $\operatorname{dist}(x,(H_{L,d,k})^c)\leqslant r$, then we have

$$\max(0,px_k-p)\leqslant p^4r^2\ \Rightarrow\ x_k\leqslant 1+p^3r^2\tag{6.317}$$

As $x\in H_{L,d,k}$, we have $x_k=\|x\|_\infty$ and we find a constant $C_\beta=C'_\beta p^{3d}$ such that the requirements of Corollary 6.16 hold with $\beta=2d$. The desired bound in (6.315) follows. We define the projections

$$P_\phi^{(3)}:=\mathbf{1}_{H_{L,d,k}}-P_\phi^{(1)}=\mathbf{1}_{\{x\in H_{L,d,k}:\ x\in(\partial H_{L,d,k})_\phi\text{ or }L/2<x_k\}}\tag{6.318}$$

and

$$P_\phi^{(4)}:=\mathbf{1}_{(H_{L,d,k})^c}-P_\phi^{(2)}=\mathbf{1}_{\{x\in(H_{L,d,k})^c:\ x\in(\partial H_{L,d,k})_\phi\text{ or }L/2<x_k<2L\}}.\tag{6.319}$$

With this at hand, we estimate (6.312) by

$$\Big|\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\Big[\mathbf{1}_{H_{V,L}}\Big(\prod_{j=1}^{p-1}\operatorname{Op}(\mathcal{D})P_{\pi(j)}\Big)\operatorname{Op}(\mathcal{D})P_\phi^{(4)}\operatorname{Op}(\psi^p\otimes\mathbb{1}_n)P_\phi^{(3)}\Big]\Big|+C_1p^{7d+1}.\tag{6.320}$$

Using the cyclic property of the trace, we estimate the trace in (6.320) by the following product of Hilbert-Schmidt norms

$$\Big\|P_\phi^{(3)}\Big(\prod_{j=1}^{p_{1,\pi}-1}\operatorname{Op}(\mathcal{D})P_0\Big)\operatorname{Op}(\mathcal{D})P_1\Big\|_2\quad\times\quad\Big\|P_1\Big(\prod_{j=p_{1,\pi}+1}^{p-1}\operatorname{Op}(\mathcal{D})P_0\Big)\operatorname{Op}(\mathcal{D})P_\phi^{(4)}\Big\|_2.\tag{6.321}$$

We split the sets corresponding to the projections $P_\phi^{(3)}$ and $P_\phi^{(4)}$ into two parts. One of distance $\frac{L}{2}$ to $H_{k-1}\setminus H_k$, the set corresponding to P_1. We estimate this part with Lemma 6.9. The other part is contained in $\left(\partial H_{L,d,k}\right)_\phi \subset \left(\partial H_{L,d,k}\right)_{\phi_m}$, for $m \in \{1, \dots, p-1\}$, and we estimate it with Lemma 6.22. In total we obtain a constant $C_2 > 0$, independent of L and p, such that (6.321) is bounded from above by

$$C_2 d^{\frac{p-1}{2}} (p-1)^{3d+2}. \tag{6.322}$$

With this we obtain a constant $C > 0$, independent of L and p, such that (6.320) and with it (6.310) are bounded from above by

$$C d^{\frac{p-1}{2}} p^{7d+1}. \tag{6.323}$$

It remains to collect the contributions from all $\pi \in \{0,1\}^{p-1}$ with $\pi \neq 0$ and the contribution from the application of Lemma 6.21 to obtain the desired bound

$$\begin{aligned}\Big| \mathrm{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \Big[\mathbf{1}_{H_{V,L}} \Big(\big(\mathbf{1}_{H_k} \operatorname{Op}(\psi\mathcal{D}) \mathbf{1}_{H_k}\big)^p - \big(\mathbf{1}_{H_{k-1}} \operatorname{Op}(\psi\mathcal{D}) \mathbf{1}_{H_{k-1}}\big)^p \Big) \mathbf{1}_{H_{L,d,k}} \\ - \mathbf{1}_{H_{V,L}} \Big(\big(\mathbf{1}_{H_k} \operatorname{Op}(\mathcal{D}) \mathbf{1}_{H_k}\big)^p - \big(\mathbf{1}_{H_{k-1}} \operatorname{Op}(\mathcal{D}) \mathbf{1}_{H_{k-1}}\big)^p \Big) \mathbf{1}_{H_{L,d,k}} \operatorname{Op}(\psi^p \otimes \mathbb{1}_n) \Big] \Big| \\ \leqslant C(2\sqrt{d})^{p-1} p^{7d+1}. \end{aligned} \tag{6.324}$$

This concludes the proof of the lemma. □

6.5.2. Proof of Theorem 6.19. We are now ready to prove Theorem 6.19 by extending the results from the previous section to entire functions.

Proof of Theorem 6.19. Let $L \geqslant 1$. We denote the pth monomial by g_p and choose a natural number $N_0 \in \mathbb{N}$ such that $m^{7d+1} \leqslant 2^m$ for all $m \geqslant N_0$. As described in the beginning of Section 6.5.1, we write

$$\begin{aligned} &\mathrm{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \Big[\sum_{V \in \mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}} X_{V,g} \Big] \\ &\qquad = 2^d \, \mathrm{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \Big[\sum_{k=1}^d c_k \mathbf{1}_{H_{V,L}} \Big(g\big(\mathbf{1}_{H_k} X \mathbf{1}_{H_k}\big) - g\big(\mathbf{1}_{H_{k-1}} X \mathbf{1}_{H_{k-1}}\big) \Big) \mathbf{1}_{H_{L,d,k}} \Big], \end{aligned} \tag{6.325}$$

with the constants $c_k := (-1)^{d-k} d \frac{(d-1)!}{(k-1)!(d-k)!}$. In the same way we write

$$\begin{aligned} &\mathrm{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \Big[\sum_{V \in \mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}} \operatorname{Op}\left(\mathcal{D}\right)_{V,g} \mathbf{1}_{H_{V,L}} \operatorname{Op}\left(g(\psi \otimes \mathbb{1}_n)\right) \Big] \\ &\quad = 2^d \, \mathrm{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n} \Big[\sum_{k=1}^d c_k \mathbf{1}_{H_{V,L}} \Big(g\big(\mathbf{1}_{H_k} \operatorname{Op}(\mathcal{D}) \mathbf{1}_{H_k}\big) - g\big(\mathbf{1}_{H_{k-1}} \operatorname{Op}(\mathcal{D}) \mathbf{1}_{H_{k-1}}\big) \Big) \\ &\qquad\qquad \times \mathbf{1}_{H_{L,d,k}} \operatorname{Op}\left(g(\psi \otimes \mathbb{1}_n)\right) \Big]. \end{aligned} \tag{6.326}$$

By the triangle inequality, it suffices to estimate the individual terms, i.e. the terms

$$\begin{aligned} &\mathbf{1}_{H_{V,L}} \Big(g\big(\mathbf{1}_{H_k} X \mathbf{1}_{H_k}\big) - g\big(\mathbf{1}_{H_{k-1}} X \mathbf{1}_{H_{k-1}}\big) \Big) \mathbf{1}_{H_{L,d,k}} \\ &\quad - \mathbf{1}_{H_{V,L}} \Big(g\big(\mathbf{1}_{H_k} \operatorname{Op}(\mathcal{D}) \mathbf{1}_{H_k}\big) - g\big(\mathbf{1}_{H_{k-1}} \operatorname{Op}(\mathcal{D}) \mathbf{1}_{H_{k-1}}\big) \Big) \mathbf{1}_{H_{L,d,k}} \operatorname{Op}\left(g(\psi)\right) =: T_g. \end{aligned} \tag{6.327}$$

The bound for polynomial test functions is given in Lemma 6.23. For the analytic function g, we obtain:

$$\left|\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[T_g\right]\right| = \left|\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\sum_{p=1}^{\infty}\omega_p T_{g_p}\right]\right| \leqslant C_1 + C_2\sum_{p=N_0}^{\infty}|\omega_p|(4\sqrt{d})^p \leqslant C_3, \tag{6.328}$$

with constants $C_1, C_2, C_3 > 0$, independent of L. Taking the limit $L \to \infty$, we obtain (6.210). This concludes the proof of the theorem. □

6.6. Local asymptotic formula

After the commutation in the last section it remains to analyse the trace of the operator

$$\sum_{V\in\mathcal{F}^{(0)}} \mathbf{1}_{H_{V,L}} \operatorname{Op}\left(\mathcal{D}\right)_{V,g}\mathbf{1}_{H_{V,L}} \operatorname{Op}\left(g(\psi\otimes\mathbb{1}_n)\right). \tag{6.329}$$

As before, all terms corresponding to the different vertices V reduce to the case $V = V_0 = \{0\}$ and $H_{V,L} = [0, L]^d$, up to suitable rotation and translation. It will be convenient to slightly modify this operator by replacing the second projection onto $H_{V,L}$ with the projection onto the slightly smaller set $(B_+)_L$, where $B_+ := \{y \in]0,\infty[^d\colon\ |y| < 1\}$. As the set $]0, L[^d\backslash(B_+)_L$ has distance L to the negative quadrant $]-\infty, 0]^d$, the structure of the operator $\operatorname{Op}\left(\mathcal{D}\right)_g$ can be used to deduce, from Lemma 6.9, that this replacement only yields an error of constant order. Due to the similarity of the proof to the one of Lemma 6.10, we will omit a proof of this fact. We also replace the first projection onto $[0, L]^d$ by the projection onto its interior $]0, L[^d$.

In order to establish an asymptotic formula, we interpret the operator

$$\mathbf{1}_{]0,L[^d} \operatorname{Op}\left(\mathcal{D}\right)_g\mathbf{1}_{(B_+)_L} \operatorname{Op}\left(g(\psi\otimes\mathbb{1}_n)\right) \tag{6.330}$$

as a multi-dimensional version of the one-dimensional localised operator studied in [Wid82] and try to adapt the one-dimensional proof to our case. In order to see the similarity of the operators, we note that both the symbols $\mathcal{D}$ and ψ only depend on momentum space. Therefore, by the unitary dilatation U_L on $L^2(\mathbb{R}^d)\otimes\mathbb{C}^n$, with $(U_L u)(x) := L^{\frac{d}{2}}u(Lx)$ for all $u \in L^2(\mathbb{R}^d)\otimes\mathbb{C}^n$, we have

$$\begin{aligned}&\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\mathbf{1}_{]0,L[^d} \operatorname{Op}\left(\mathcal{D}\right)_g\mathbf{1}_{(B_+)_L} \operatorname{Op}\left(g(\psi\otimes\mathbb{1}_n)\right)\right]\\&\qquad= \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\mathbf{1}_{]0,1[^d} \operatorname{Op}\left(\mathcal{D}\right)_g\mathbf{1}_{B_+} \operatorname{Op}_L\left(g(\psi\otimes\mathbb{1}_n)\right)\right],\end{aligned} \tag{6.331}$$

where we used the fact that the symbol $\mathcal{D}$ is homogeneous of degree 0 and therefore $\operatorname{Op}_L(\mathcal{D}) = \operatorname{Op}(\mathcal{D})$, where Op_L is the operator with semi-classical parameter L, see Section 2.1. Following the proof of the one-dimensional case in [Wid82], the first step would be to determine the integral kernel of the operator $\operatorname{Op}\left(\mathcal{D}\right)_g$. In [Wid82] the kernel is derived explicitly with the use of the Mellin transform and its interaction with the Hilbert transform, which is the integral kernel of $\operatorname{Op}(\mathcal{D})$ in dimension 1. Unfortunately, it seems difficult to generalise this step to our multi-dimensional case. This is on the one hand due to the far more complicated structure of $\operatorname{Op}\left(\mathcal{D}\right)_g$ in higher dimensions and on the other hand due to the fact that, instead of simply being the Hilbert transform, the integral kernel of $\operatorname{Op}(\mathcal{D})$ is then composed of its more complicated multi-dimensional generalisations, the Riesz transforms. The alternative chosen here is to establish the properties of the integral kernel, which are required for the second step, the local asymptotic formula, by hand. Unfortunately, we are only able to do this in the special case that g is given by g_2 the monomial of second degree. This is the reason for the restriction on g in Theorem 6.3. Establishing these properties for g_2 is the content of the following section.

6.6.1. Integral kernel properties for the second moment.

Lemma 6.24. *Denote by g_2 the second monomial and let $K : \mathbb{R}^d \times \mathbb{R}^d \longrightarrow \mathbb{C}^n$ be the corresponding integral kernel of the operator $\mathrm{Op}\left(\mathcal{D}\right)_{g_2}$. Then K is continuous on $]0,\infty[^d \times]0,\infty[^d$, homogeneous of degree $-d$, has non-vanishing trace on $]0,\infty[^d \times]0,\infty[^d$ and satisfies the bound*

$$\left|\mathrm{tr}_{\mathbb{C}^n}\left[K(z,z) - K(x,z)\right]\right| \leqslant C_d\sqrt{|x-z|}\,\left|\mathrm{tr}_{\mathbb{C}^n}\left[K(x,z)\right]\right|, \tag{6.332}$$

for every $z \in]0,\infty[^d$ with $|z| = 1$, $x \in [z-\delta_z, z+\delta_z]^d$, with $\delta_z := \min_{j=1,\dots,d}\left(\frac{z_j}{2}\right)^2$, and a constant $C_d > 0$, which only depends on the dimension d. Furthermore, K satisfies the bound

$$\|K(x,z)\|_2 \leqslant C_K\left(|x||z|\right)^{-\frac{d}{2}}, \tag{6.333}$$

for every $x, z \in]0,\infty[^d$, with a constant C_K independent of x and z.

PROOF. We begin with the homogeneity of K. We write out the operator $\mathbf{1}_{]0,\infty[^d}\,\mathrm{Op}\left(\mathcal{D}\right)_{g_2}\mathbf{1}_{]0,\infty[^d}$

$$\begin{aligned}\mathbf{1}_{\mathbb{R}^d_+}\,\mathrm{Op}\left(\mathcal{D}\right)_{g_2}\mathbf{1}_{]0,\infty[^d} &= \sum_{k=0}^{d}(-1)^k \sum_{\mathcal{M}\subseteq\{1,\dots,d\}\,:\,|\mathcal{M}|=k} \mathbf{1}_{]0,\infty[^d}\left(\mathbf{1}_{H_\mathcal{M}}\mathrm{Op}(\mathcal{D})\mathbf{1}_{H_\mathcal{M}}\right)^2\mathbf{1}_{]0,\infty[^d}\\ &= (-1)^d\mathbf{1}_{]0,\infty[^d}\,\mathrm{Op}(\mathcal{D})\mathbf{1}_{]-\infty,0[^d}\,\mathrm{Op}(\mathcal{D})\mathbf{1}_{]0,\infty[^d}.\end{aligned} \tag{6.334}$$

Therefore, the kernel at some point $(x,z) \in]0,\infty[^d \times]0,\infty[^d$ can be written as

$$K(x,z) = (-1)^d \int_{]-\infty,0[^d} K_0(x,y)K_0(y,z)\,\mathrm{d}y, \tag{6.335}$$

with K_0 being the kernel of $\mathrm{Op}(\mathcal{D})$. The homogeneity of K follows from the homogeneity of K_0 and substitution in the variable y.

With the definition of K_0, equation (6.335) immediately yields that the trace of K is either strictly positive or strictly negative on $]0,\infty[^d \times]0,\infty[^d$.

We continue with the continuity of the kernel. We again write

$$K(x,z) = (-1)^d \int_{]-\infty,0[^d} K_0(x,y)K_0(y,z)\,\mathrm{d}y. \tag{6.336}$$

The function $K_0(x,y)K_0(y,z)$ is continuous on $]0,\infty[^d \times]0,\infty[^d$ for every $y \in]-\infty,0[^d$ and integrable for fixed $(x_0,z_0) \in]0,\infty[^d \times]0,\infty[^d$. We choose $\frac{\min(|x_0|,|z_0|)}{2} > \delta > 0$ such that additionally $B_\delta(x_0,z_0) \subset]0,\infty[^d \times]0,\infty[^d$. With the bound (6.45), we obtain

$$\|K_0(x,y)K_0(y,z)\|_2 \leqslant C_{K_0}^2\frac{1}{|x-y|^d|y-z|^d}. \tag{6.337}$$

Let $(x,z) \in B_\delta(x_0,z_0)$. Then, by the choice of δ, we have

$$\frac{|x_0-y|}{|x-y|} \leqslant 1 + \frac{|x-x_0|}{|x-y|} \leqslant 2, \tag{6.338}$$

for arbitrary $y \in]-\infty,0[^d$. We bound $\frac{|y-z_0|}{|y-z|}$ in the same way and obtain the following bound for the right-hand side of (6.337)

$$4^d C_{K_0}^2\frac{1}{|x_0-y|^d|y-z_0|^d}. \tag{6.339}$$

As this is integrable on $]-\infty,0]^d$, the continuity of the Kernel K follows.

We now turn towards the proof of the bound (6.332). We estimate

$$\begin{aligned}\left|\operatorname{tr}_{\mathbb{C}^n}[K(z,z)-K(x,z)]\right| &\leqslant \left(\tfrac{c_d}{2}\right)^2\sum_{j=1}^d\int_{]-\infty,0[^d}\left|\frac{z_j-y_j}{|z-y|^{d+1}}-\frac{x_j-y_j}{|x-y|^{d+1}}\right|\frac{z_j-y_j}{|y-z|^{d+1}}\,\mathrm{d}y\\ &=\left(\tfrac{c_d}{2}\right)^2\sum_{j=1}^d\int_{]-\infty,0[^d}\left|\frac{(z_j-y_j)|x-y|^{d+1}}{(x_j-y_j)|z-y|^{d+1}}-1\right|\frac{x_j-y_j}{|x-y|^{d+1}}\frac{z_j-y_j}{|y-z|^{d+1}}\,\mathrm{d}y,\end{aligned} \tag{6.340}$$

where we used that $x_j-y_j>0$, for all $y\in]-\infty,0[^d$ and $j\in\{1,\dots,d\}$, as $x\in[z-\delta_z,z+\delta_z]^d\subset]0,\infty[^d$. We recall $c_d=\frac{\Gamma[(d+1)/2]}{\pi^{(d+1)/2}}$. With the triangle inequality we obtain

$$\tfrac{z_j-y_j}{x_j-y_j}\in\left[1-\tfrac{|x_j-z_j|}{x_j-y_j},1+\tfrac{|x_j-z_j|}{x_j-y_j}\right]\subseteq\left[1-\tfrac{\sqrt{\delta_z|x-z|}}{\sqrt{\delta_z}},1+\tfrac{\sqrt{\delta_z|x-z|}}{\sqrt{\delta_z}}\right], \tag{6.341}$$

where, in the last step, we used that $x\in[z-\delta_z,z+\delta_z]^d$, $|x_j-z_j|\leqslant|x-z|$ and $x_j-y_j\geqslant\sqrt{\delta_z}$, for all $y\in]-\infty,0[^d$, by the definition of δ_z. The triangle inequality also yields

$$\tfrac{|x-y|}{|z-y|}\in\left[1-\tfrac{|x-z|}{|z-y|},1+\tfrac{|x-z|}{|z-y|}\right]\subseteq\left[1-|x-z|,1+|x-z|\right], \tag{6.342}$$

where we used that $|z-y|\geqslant 1$ for all $y\in]-\infty,0[^d$, as $|z|=1$. With these two estimates, we find a constant $C_d>0$, only depending on the dimension d, such that the right-hand side of (6.340) is bounded from above by

$$C_d\sqrt{|x-z|}\left(\tfrac{c_d}{2}\right)^2\sum_{j=1}^d\int_{]-\infty,0[^d}\frac{x_j-y_j}{|x-y|^{d+1}}\frac{z_j-y_j}{|y-z|^{d+1}}\,\mathrm{d}y=C_d\sqrt{|x-z|}\,\left|\operatorname{tr}_{\mathbb{C}^n}[K(x,z)]\right|. \tag{6.343}$$

This concludes the proof of the bound (6.332).

It remains to verify the bound (6.333). We again have

$$K(x,z)=(-1)^d\int_{]-\infty,0[^d}K_0(x,y)K_0(y,z)\,\mathrm{d}y. \tag{6.344}$$

With the bound (6.45), we obtain

$$\|K(x,z)\|_2\leqslant C_{K_0}^2\int_{]-\infty,0[^d}\frac{1}{|x-y|^d|y-z|^d}\,\mathrm{d}y=C_{K_0}^2\int_{]0,\infty[^d}\frac{1}{|x+y|^d|y+z|^d}\,\mathrm{d}y. \tag{6.345}$$

Using the fact that x,y,z are all in the same quadrant, as well as the inequality $\sqrt{a+b}\geqslant\frac{1}{\sqrt{2}}(\sqrt{a}+\sqrt{b})$ for $a,b>0$, we see that

$$|x+y||y+z|\geqslant\frac{1}{2}(|x|+|y|)(|y|+|z|). \tag{6.346}$$

Therefore, the right-hand side of (6.345) is bounded from above by

$$2^dC_{K_0}^2\int_{]0,\infty[^d}\frac{1}{[(|x|+|y|)(|y|+|z|)]^d}\,\mathrm{d}y\leqslant 2^dC_{K_0}^2\int_{]0,\infty[^d}\frac{1}{(|x||z|+|y|^2)^d}\,\mathrm{d}y. \tag{6.347}$$

Introducing spherical coordinates, we write this as

$$C_{K_0}^2|S^{d-1}|\int_0^\infty\frac{r^{d-1}}{(|x||z|+r^2)^d}\,\mathrm{d}r\leqslant C_{K_0}^2|S^{d-1}|\int_0^\infty\frac{r}{(|x||z|+r^2)^{\frac{d+2}{2}}}\,\mathrm{d}r\leqslant C_K(|x||z|)^{-\frac{d}{2}}, \tag{6.348}$$

where the constant $C_K>0$ is independent of x and z. This concludes the proof of the bound (6.333) and with it the proof of the lemma. □

6.6.2. A local asymptotic formula. We now prove a local asymptotic formula in a similar way as done in the one-dimensional case in [Wid82]. We employ a similar scaling argument as in [Wid82] and use the homogeneity of the integral kernel. But instead of reducing the positive half-axis $]0,\infty[$ to the single point $\{1\}$, we reduce the positive quadrant $]0,\infty[^d$ to the $(d-1)$-dimensional set $S_+^{d-1} = \{y \in]0,\infty[^d : \ |y| = 1\}$. The higher-dimensional nature of this reduced set adds some additional challenges to the proof and leads to more extensive requirements. In particular, we require that the trace of the integral kernel of the operator does not vanish. This requirement could be easily avoided in the one-dimensional case.

Theorem 6.25. *Let X be an integral operator on $L^2(\mathbb{R}^d)\otimes\mathbb{C}^n$. Let its integral kernel K be continuous on $]0,\infty[^d\times]0,\infty[^d$, homogeneous of degree $-d$, have non-vanishing trace on $]0,\infty[^d\times]0,\infty[^d$ and satisfy the bounds* (6.332) *and* (6.333)*. Then we have*

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\mathbf{1}_{]0,1[^d}X\mathbf{1}_{B_+}\operatorname{Op}_L(\sigma\otimes\mathbb{1}_n)\right] = \log L\ \sigma(0)\int_{S_+^{d-1}}\operatorname{tr}_{\mathbb{C}^n}[K(y,y)]\,\mathrm{d}y + O(1), \tag{6.349}$$

as $L\to\infty$.

Proof. The kernel of $\mathbf{1}_{]0,1[^d}X\mathbf{1}_{B_+}\operatorname{Op}_L(\sigma\otimes\mathbb{1}_n)$ at a point $(x,y)\in]0,1[^d\times\mathbb{R}^d$ is given by

$$\frac{L^d}{(2\pi)^d}\int_{B_+}\int_{\mathbb{R}^d}K(x,z)e^{\mathrm{i}L\xi(z-y)}\sigma(\xi)\,\mathrm{d}\xi\,\mathrm{d}z. \tag{6.350}$$

As this is continuous, we compute the trace on the left-hand side of (6.349) by integrating this kernel along the diagonal, i.e. we have

$$\begin{aligned}&\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\mathbf{1}_{]0,1[^d}X\mathbf{1}_{B_+}\operatorname{Op}_L(\sigma\otimes\mathbb{1}_n)\right]\\ &\qquad = \frac{L^d}{(2\pi)^d}\int_{]0,1[^d}\int_{B_+}\int_{\mathbb{R}^d}\operatorname{tr}_{\mathbb{C}^n}[K(x,z)]e^{\mathrm{i}L\xi(z-x)}\sigma(\xi)\,\mathrm{d}\xi\,\mathrm{d}z\,\mathrm{d}x.\end{aligned} \tag{6.351}$$

We now need to evaluate this asymptotically as $L\to\infty$. The integrand on the right-hand side of (6.351) is clearly integrable. Hence, we can change the order of integration by Fubini's Theorem. We first introduce spherical coordinates in the variable z and rewrite the right-hand side of (6.351) as

$$\frac{L^d}{(2\pi)^d}\int_{S_+^{d-1}}\int_{]0,1[^d}\int_0^1\int_{\mathbb{R}^d}r^{d-1}\operatorname{tr}_{\mathbb{C}^n}[K(x,ry)]e^{\mathrm{i}L\xi(ry-x)}\sigma(\xi)\,\mathrm{d}\xi\,\mathrm{d}r\,\mathrm{d}x\,\mathrm{d}y. \tag{6.352}$$

Let now $\phi_y:\mathbb{R}^d\to\mathbb{R}$ be measurable functions, for every $y\in S_+^{d-1}$. We begin by estimating the expression

$$\frac{L^d}{(2\pi)^d}\int_{S_+^{d-1}}\int_{]0,1[^d}\int_0^1\int_{\mathbb{R}^d}r^{d-1}\operatorname{tr}_{\mathbb{C}^n}[K(x,ry)]\left[1-\phi_y\left(\tfrac{x}{r}\right)\right]e^{\mathrm{i}L\xi(ry-x)}\sigma(\xi)\,\mathrm{d}\xi\,\mathrm{d}r\,\mathrm{d}x\,\mathrm{d}y. \tag{6.353}$$

As we have $\sigma\in C_c^\infty(\mathbb{R}^d)$, integrating by parts $d+1$ times yields the bound

$$\left|\int_{\mathbb{R}^d}e^{\mathrm{i}L\xi(ry-x)}\sigma(\xi)\,\mathrm{d}\xi\right|\leqslant C_\sigma(1+L|ry-x|)^{-d-1}, \tag{6.354}$$

with a constant $C_\sigma>0$ independent of L. With this, the absolute value of (6.353) is bounded from above by

$$\frac{L^dC_\sigma}{(2\pi)^d}\int_{S_+^{d-1}}\int_{]0,\infty[^d}\int_0^1 r^{d-1}\big|\operatorname{tr}_{\mathbb{C}^n}[K(x,ry)]\big|\big|1-\phi_y\left(\tfrac{x}{r}\right)\big|(1+L|ry-x|)^{-d-1}\,\mathrm{d}r\,\mathrm{d}x\,\mathrm{d}y. \tag{6.355}$$

With the substitution $x \mapsto rx$ and the homogeneity of K this is equal to

$$\frac{L^d C_\sigma}{(2\pi)^d} \int_{S_+^{d-1}} \int_{]0,\infty[^d} \int_0^1 r^{d-1} \big| \operatorname{tr}_{\mathbb{C}^n}[K(x,y)] \big| \big| 1 - \phi_y(x) \big| (1 + Lr|y-x|)^{-d-1} \, \mathrm{d}r \, \mathrm{d}x \, \mathrm{d}y. \tag{6.356}$$

Carrying out the integration in the variable r, we obtain

$$\begin{aligned} \int_0^1 r^{d-1}(1+Lr|y-x|)^{-d-1} \, \mathrm{d}r &\leqslant \int_0^\infty r^{d-1}(1+Lr|y-x|)^{-d-1} \, \mathrm{d}r \\ &= \frac{r^d (Lr|y-x|+1)^{-d}}{d} \Bigg|_{r=0}^{r=\infty} = \frac{1}{dL^d|y-x|^d} \end{aligned} \tag{6.357}$$

and therefore (6.356) is bounded from above by

$$\frac{C_\sigma}{d(2\pi)^d} \int_{S_+^{d-1}} \int_{]0,\infty[^d} \big| \operatorname{tr}_{\mathbb{C}^n}[K(x,y)] \big| \big| 1 - \phi_y(x) \big| |y-x|^{-d} \, \mathrm{d}x \, \mathrm{d}y. \tag{6.358}$$

Due to the bound (6.333), we have $\big| \operatorname{tr}_{\mathbb{C}^n}[K(x,y)] \big| \leqslant C_K |x|^{\frac{-d}{2}}$ for all $x \in]0,\infty[^d$. Choosing $\delta_y := \big(\frac{\min_{1\leqslant j\leqslant d} y_j}{2}\big)^2$, we see that $[y-\delta_y, y+\delta_y]^d \subset]0,\infty[^d$ and therefore $\operatorname{tr}_{\mathbb{C}^n}[K(x,y)] \neq 0$ for all $x \in [y-\delta_y, y+\delta_y]^d$, by assumption. We choose the functions

$$\phi_y(x) := \omega_y(x) \frac{\operatorname{tr}_{\mathbb{C}^n}[K(y,y)]}{\operatorname{tr}_{\mathbb{C}^n}[K(x,y)]} := 1_{[y-\delta_y, y+\delta_y]^d}(x) \frac{\operatorname{tr}_{\mathbb{C}^n}[K(y,y)]}{\operatorname{tr}_{\mathbb{C}^n}[K(x,y)]}. \tag{6.359}$$

With these functions and the bound (6.332), the integral in the variable x in (6.358) is bounded by a constant, which is independent of y, times

$$\begin{aligned} C_K \int_{]0,1/2]^d} |x|^{\frac{-d}{2}} \, \mathrm{d}x &+ \int_{]0,2]^d \setminus ([y-\delta_y, y+\delta_y]^d \cup]0,1/2]^d)} |y-x|^{-d} \, \mathrm{d}x \\ &+ C_d \int_{[y-\delta_y, y+\delta_y]^d} |y-x|^{-d+1/2} \, \mathrm{d}x + C_K \int_{]0,\infty[^d \setminus]0,2]^d} |x|^{\frac{-3d}{2}} \, \mathrm{d}x. \end{aligned} \tag{6.360}$$

This is bounded from above by $C_1 + C_2 |\log(\delta_y)|$, where the constants $C_1, C_2 > 0$ are independent of y and L. Carrying out the remaining integration in the variable y in (6.358), we see that (6.358) is bounded independently of L.

Hence, we reduced the trace in (6.349) to

$$\frac{L^d}{(2\pi)^d} \int_{S_+^{d-1}} \int_{]0,1[^d} \int_0^1 \int_{\mathbb{R}^d} r^{d-1} \operatorname{tr}_{\mathbb{C}^n}[K(x,ry)] \phi_y\big(\tfrac{x}{r}\big) e^{\mathrm{i}L\xi(ry-x)} \sigma(\xi) \, \mathrm{d}\xi \, \mathrm{d}r \, \mathrm{d}x \, \mathrm{d}y \tag{6.361}$$

up to an error term of constant order. With the homogeneity of K we obtain

$$\operatorname{tr}_{\mathbb{C}^n}[K(x,ry)] \phi_y\big(\tfrac{x}{r}\big) = r^{-d} \omega_y\big(\tfrac{x}{r}\big) \operatorname{tr}_{\mathbb{C}^n}[K(y,y)] \tag{6.362}$$

and with this, (6.361) reads

$$\frac{L^d}{(2\pi)^d} \int_{S_+^{d-1}} \operatorname{tr}_{\mathbb{C}^n}[K(y,y)] \int_{\mathbb{R}^d} \int_0^1 r^{-1} \omega_y\big(\tfrac{x}{r}\big) \int_{\mathbb{R}^d} \sigma(\xi) e^{\mathrm{i}L\xi(ry-x)} \, \mathrm{d}\xi \, \mathrm{d}r \, \mathrm{d}x \, \mathrm{d}y. \tag{6.363}$$

Here, we used that $\operatorname{supp}\phi_y \subset]0,1[^d$ and $r \leqslant 1$. Translating the variable x by ry and using the definition of ω_y, this is equal to

$$\frac{L^d}{(2\pi)^d} \int_{S_+^{d-1}} \operatorname{tr}_{\mathbb{C}^n}[K(y,y)] \int_{\mathbb{R}^d} \int_0^1 r^{-1} 1_{[-\delta_y r, \delta_y r]^d}(x) \int_{\mathbb{R}^d} \sigma(\xi) e^{-\mathrm{i}L\xi x} \, \mathrm{d}\xi \, \mathrm{d}r \, \mathrm{d}x \, \mathrm{d}y. \tag{6.364}$$

Substituting $x \mapsto \frac{x}{L}$ and carrying out the integration in the variable ξ, this is equal to

$$(2\pi)^{-\frac{d}{2}} \int_{S_+^{d-1}} \operatorname{tr}_{\mathbb{C}^n}[K(y,y)] \int_{\mathbb{R}^d} \hat{\sigma}(x) \int_0^1 1_{[-L\delta_y r, L\delta_y r]^d}(x) \frac{\mathrm{d}r}{r} \,\mathrm{d}x \,\mathrm{d}y. \tag{6.365}$$

We now consider the integral in the variable r. We see that it vanishes for $\|x\|_\infty \geqslant L\delta_y$. Therefore, we have

$$\begin{aligned} \int_0^1 1_{[-L\delta_y r, L\delta_y r]^d}(x) \frac{\mathrm{d}r}{r} &= 1_{\{x\in\mathbb{R}^d \quad \|x\|_\infty < L\delta_y\}} \int_{\frac{\|x\|_\infty}{L\delta_y}}^1 \frac{\mathrm{d}r}{r} \\ &= 1_{\{x\in\mathbb{R}^d \quad \|x\|_\infty < L\delta_y\}} [\log L + \log \delta_y - \log \|x\|_\infty]. \end{aligned} \tag{6.366}$$

With this (6.365) reads

$$(2\pi)^{-\frac{d}{2}} \int_{S_+^{d-1}} \operatorname{tr}_{\mathbb{C}^n}[K(y,y)] \int_{\mathbb{R}^d} \hat{\sigma}(x) 1_{\{x\in\mathbb{R}^d \quad \|x\|_\infty < L\delta_y\}} [\log L + \log \delta_y - \log \|x\|_\infty] \,\mathrm{d}x \,\mathrm{d}y. \tag{6.367}$$

Rewriting this as

$$\begin{aligned} &\log L \; \sigma(0) \int_{S_+^{d-1}} \operatorname{tr}_{\mathbb{C}^n}[K(y,y)] \,\mathrm{d}y \\ &\quad + \sigma(0) \int_{S_+^{d-1}} \log \delta_y \operatorname{tr}_{\mathbb{C}^n}[K(y,y)] \,\mathrm{d}y \\ &\quad - (2\pi)^{-\frac{d}{2}} \int_{S_+^{d-1}} \operatorname{tr}_{\mathbb{C}^n}[K(y,y)] \int_{\mathbb{R}^d} \hat{\sigma}(x) 1_{\{x\in\mathbb{R}^d \quad \|x\|_\infty < L\delta_y\}} \log \|x\|_\infty \,\mathrm{d}x \,\mathrm{d}y \\ &\quad - (2\pi)^{-\frac{d}{2}} \int_{S_+^{d-1}} [\log L + \log \delta_y] \operatorname{tr}_{\mathbb{C}^n}[K(y,y)] \int_{\mathbb{R}^d} \hat{\sigma}(x) 1_{\{x\in\mathbb{R}^d \quad \|x\|_\infty \geqslant L\delta_y\}} \,\mathrm{d}x \,\mathrm{d}y, \end{aligned} \tag{6.368}$$

we have found the desired asymptotic coefficient. It only remains to verify that the other terms in (6.368) are of sufficiently low order. By the definition of δ_y and the bound (6.333), the term in the second line of (6.368) is finite and it is clearly of constant order. As $\hat{\sigma}$ is a Schwartz function, the term in the third line of (6.368) is also finite and of constant order. For the terms in the fourth line of (6.368), we also use that $\hat{\sigma}$ is Schwartz to obtain the bound

$$\left| \int_{\mathbb{R}^d} \hat{\sigma}(x) 1_{\{x\in\mathbb{R}^d \quad \|x\|_\infty \geqslant L\delta_y\}} \,\mathrm{d}x \right| \leqslant \frac{C'_\sigma}{\left(1 + L\delta_y\right)^\alpha}, \tag{6.369}$$

with $C'_\sigma > 0$, independent of L and δ_y, and $0 < \alpha < \frac{1}{2}$. This guarantees that the terms in the fourth line of (6.368) are both finite and of lower than constant order. With this, we see that (6.368) equals

$$\log L \; \sigma(0) \int_{S_+^{d-1}} \operatorname{tr}_{\mathbb{C}^n}[K(y,y)] \,\mathrm{d}y + O(1), \tag{6.370}$$

as $L \to \infty$. This concludes the proof of the theorem. □

6.6.3. Proof of Theorem 6.3. We are now in a position to prove the second main result of the present chapter, Theorem 6.3, by combining the results of this section with the previous sections. For polynomials of degree 3, we make use of the matrix structure of the Dirac matrices.

Proof of Theorem 6.3. In the case that h is of degree 1, there is nothing to show. We start with the case $h = g_2$. By Theorem 6.8 we have

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[g_2\big(\mathbf{1}_{\Lambda_L}\operatorname{Op}(\psi\mathcal{D})\mathbf{1}_{\Lambda_L}\big)\right] = \sum_{m=0}^{d-1}(2L)^{d-m}A_{m,g_2,b}$$
$$+\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\sum_{V\in\mathcal{F}^{(0)}}\mathbf{1}_{H_{V,L}}\operatorname{Op}(\psi\mathcal{D})_{V,g_2}\right]+O(1), \quad (6.371)$$

as $L\to\infty$. It remains to compute the trace on the right-hand side. By Theorem 6.19 and the discussion at the beginning of Section 6.6 we have for $V = V_0 = \{0\}$

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\mathbf{1}_{H_{V_0,L}}\operatorname{Op}(\psi\mathcal{D})_{V_0,g_2}\right] = \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\mathbf{1}_{]0,1[^d}\operatorname{Op}(\mathcal{D})_{g_2}\mathbf{1}_{B_+}\operatorname{Op}_L(\psi^2\otimes\mathbb{1}_n)\right]+O(1), \quad (6.372)$$

as $L\to\infty$. By Lemma 6.24, the operator $\operatorname{Op}(\mathcal{D})_{g_2}$ fulfils the requirements of Theorem 6.25. An application of Theorem 6.25 yields

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\mathbf{1}_{]0,1[^d}\operatorname{Op}(\mathcal{D})_{g_2}\mathbf{1}_{B_+}\operatorname{Op}_L(\psi^2\otimes\mathbb{1}_n)\right] = \log L\int_{S_+^{d-1}}\operatorname{tr}_{\mathbb{C}^n}[K_{g_2}(y,y)]\,\mathrm{d}y+O(1), \quad (6.373)$$

as $L\to\infty$, where K_{g_2} is the integral kernel of the operator $\operatorname{Op}(\mathcal{D})_{g_2}$. Collecting the contributions for all $V\in\mathcal{F}^{(0)}$ concludes the proof of the Theorem in the case $h = g_2$.

We now turn to the third moment, i.e. the case $h = g_3$. The results from Sections 6.3 and 6.5 apply to analytic functions, in particular also in the case $h = g_3$. Therefore, it only remains to justify an application of the results from Section 6.6. As the Dirac matrices have vanishing trace, only the terms where the identity matrix occurs once or thrice contribute to the trace. Due to the structure of the operator $\operatorname{Op}\left(\mathcal{D}\right)_{g_3}$, the case where the identity occurs thrice vanishes. Therefore, we have

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\mathbf{1}_{]0,1[^d}\operatorname{Op}\left(\mathcal{D}\right)_{g_3}\mathbf{1}_{B_+}\operatorname{Op}_L(\psi^3\otimes\mathbb{1}_n)\right]$$
$$=\frac{3}{2}\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\mathbf{1}_{]0,1[^d}\operatorname{Op}\left(\mathcal{D}\right)_{g_2}\mathbf{1}_{B_+}\operatorname{Op}_L(\psi^3\otimes\mathbb{1}_n)\right]. \quad (6.374)$$

As $\psi^3(0) = \psi^2(0) = 1$, an application of Theorem 6.25 yields

$$\operatorname{tr}_{L^2(\mathbb{R}^d)\otimes\mathbb{C}^n}\left[\mathbf{1}_{]0,1[^d}\operatorname{Op}(\mathcal{D})_{g_3}\mathbf{1}_{B_+}\operatorname{Op}_L(\psi^3\otimes\mathbb{1}_n)\right] = \frac{3}{2}\log L\int_{S_+^{d-1}}\operatorname{tr}_{\mathbb{C}^n}[K_{g_2}(y,y)]\,\mathrm{d}y+O(1), \quad (6.375)$$

as $L\to\infty$. Using the structure of the Dirac matrices again, we see that

$$\frac{3}{2}\operatorname{tr}_{\mathbb{C}^n}[K_{g_2}(y,y)] = \operatorname{tr}_{\mathbb{C}^n}[K_{g_3}(y,y)], \quad (6.376)$$

which concludes the proof of the Theorem in the case $h = g_3$. The result for arbitrary polynomials of degree at most three follows by linearity. □

Nomenclature

$\mathbb{N}$	The natural numbers, without zero
$\mathbb{N}_0$	$= \mathbb{N} \cup \{0\}$
d	The spatial dimension, $d \in \mathbb{N}$
$\mathbb{R}^d$	d-dimensional Euclidian space
L	Scaling parameter; we always assume $L > 0$
Λ_L	$= \{Lx \in \mathbb{R}^d : \ x \in \Lambda \subset \mathbb{R}^d\}$, scaled version of the region $\Lambda \subset \mathbb{R}^d$
E_F	The Fermi energy, $E_F \in \mathbb{R}$
m	The (physical) mass, $m \geqslant 0$
$\mathbb{Z}$	The integers
$\mathbb{T}$	The torus
log	The natural logarithm
det	The determinant
$\mathcal{S}(\mathbb{R}^d)$	The Schwartz functions on $\mathbb{R}^d$
$\mathrm{tr}_{\mathcal{H}}[X]$	The trace of an operator X acting on the separable Hilbert space $\mathcal{H}$ (either trace class or sign-definite)
$\mathbb{R}_+$	$= [0, \infty[$; the non-negative real numbers
$\mathbb{C}^{n\times n}$	The set of complex-valued $n \times n$ square matrices
$C(U)$	The space of complex-valued continuous functions on $U \subseteq \mathbb{R}^d$ open.
$C^k(U)$	The space of complex-valued k-times continuously differentiable functions on $U \subseteq \mathbb{R}^d$ open, for $k \in \mathbb{N} \cup \{\infty\}$.
$C_c^k(U)$	The space of functions $f \in C^k(U)$ with compact support
$C_b^\infty(\mathbb{R}^d)$	The functions $f \in C^\infty(\mathbb{R}^d)$ such that f and all its partial derivatives are bounded
$\partial\Omega$	The boundary (in $\mathbb{R}^d$) of a set $\Omega \subset \mathbb{R}^d$
$\overline{\Omega}$	The closure (in $\mathbb{R}^d$) of a set $\Omega \subset \mathbb{R}^d$
Ω°	The interior (in $\mathbb{R}^d$) of a set $\Omega \subset \mathbb{R}^d$
Ω^c	The complement (in $\mathbb{R}^d$) of a set $\Omega \subset \mathbb{R}^d$
1_Ω	The indicator function (on $\mathbb{R}^d$) of a set $\Omega \subset \mathbb{R}^d$; Also the operator of multiplication with this indicator function on $L^2(\mathbb{R}^d)$
$\mathbb{1}_n$	The $n \times n$ unit matrix
$\mathbf{1}_\Omega$	$= 1_\Omega \otimes \mathbb{1}_n$; The indicator function on $\mathbb{R}^d \otimes \mathbb{C}^n$ of a set $\Omega \subset \mathbb{R}^d$; Also the operator of multiplication with said indicator function on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$

$\mathrm{Op}_L(A)$	The (pseudo-differential) operator (PDO) with semi-classical scaling parameter L of a suitable (matrix-valued) symbol A, depending on a single variable
$\mathrm{Op}_L^l(A)$	The left-quantisation of the PDO with symbol A
$\mathrm{Op}_L^r(A)$	The right-quantisation of the PDO with symbol A
$\mathrm{Op}_L^{lr}(A)$	The PDO with matrix-valued amplitude A
Re	The self-adjoint (real) part of a number, matrix or linear operator
1_{E_F}	$= 1_{\{x\in\mathbb{R}:\ x<E_F\}}$, the Fermi projection
$\dim(U)$	The dimension of a vector space U or, in the case that $U \subset \mathbb{R}^d$ is not a vector space, the dimension of the smallest affine subspace of $\mathbb{R}^d$ which contains U
$B_R(x)$	The d-dimensional open ball of radius $R > 0$ centred about the point $x \in \mathbb{R}^d$
S^{d-1}	$= \partial B_1(0)$, the $d-1$ dimensional unit sphere
$\mathcal{F}$	The Fourier transform on $L^2(\mathbb{R}^d)$
$\hat{f}$	The Fourier transform of a function f
$\check{f}$	The inverse Fourier transform of a function f
$\nu_{\partial\Omega}$	The vector field of exterior unit normals in $\mathbb{R}^d$ to the boundary $\partial\Omega$
$\mathrm{d}S$	The $(d-1)$-dimensional surface measure induced by Lebesgue measure in $\mathbb{R}^d$ for a given surface
∂_k	Partial differentiation with respect to the kth Cartesian coordinate
$\lvert\alpha\rvert$	$= \sum_{j=1}^d \lvert\alpha_j\rvert$ for a given multi-index $\alpha \in \mathbb{N}_0^d$
D	The free Dirac operator, densely defined in $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$ the Hilbert space of square-integrable vector-valued functions; also used for the symbol of the corresponding differential operator, i.e. $\mathrm{Op}(D) = D$
$\lfloor r \rfloor$	The largest integer not exceeding $r \in \mathbb{R}$
X^*	The adjoint of an operator X
δ_{jk}	The Kronecker delta
E	The energy momentum relation in the free Dirac equation given by $\xi \mapsto E(\xi) = \sqrt{m^2 + \xi^2}$
$\chi_{E_F}^{(b)}$	A smoothly truncated version of the Fermi projection, depending on the cut-off parameter $b \geqslant 0$
$\mathrm{dist}(\Omega, \Omega')$	The Euclidian distance between the sets $\Omega, \Omega' \subset \mathbb{R}^d$
$\mathrm{dist}(x, \Omega)$	$= \mathrm{dist}(\{x\}, \Omega)$ for $x \in \mathbb{R}^d$
$\mathcal{D}$	The symbol given by the Fermi projection $1_0(D)$ of the massless Dirac operator at Fermi energy zero
g_p	The pth monomial
$\lVert X\rVert_q$	The Schatten–von Neumann q (quasi)-norm for an operator X and $q \in]0, \infty[$
$\mathrm{supp}\, f$	The support of a function f
$\mathrm{ran}\, f$	The range of a function
$\mathcal{S}_p$	The symmetric group on the set $\{1, \dots, p\}$, $p \in \mathbb{N}$
$1_{\mathcal{H}}$	The identity on a given Hilbert space $\mathcal{H}$
$\lVert x\rVert_\infty$	$= \max_{1\leqslant k\leqslant d} \lvert x_k\rvert$ for $x \in \mathbb{R}^d$
$\lVert f\rVert_\infty$	The supremum norm of a function $f : \mathbb{R}^d \to \mathbb{C}$
Q_x	The closed unit cube centred about $x \in \mathbb{R}^d$

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Eidesstattliche Versicherung

(Siehe Promotionsordnung vom 12.07.11, § 8 Abs. 2 Pkt. 5.)

Hiermit erkläre ich an Eidesstatt, dass die Dissertation von mir selbstständig, ohne unerlaubte Beihilfe angefertigt ist.

Leon Bollmann

München, den 30.09.2025	Leon Bollmann
Ort, Datum	Unterschrift Doktorand/in