Spectral asymptotics associated with Dirac-type operators

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Spectral asymptotics associated with Dirac-type operators

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This thesis is concerned first with a non-compact variation of Connes' trace theorem, which demonstrated that the Dixmier trace extends the notion of Lebesgue integration on a compact manifold. To obtain the variation, we develop a new ζ-residue formula, which is proved by an innovative approach using double operator integrals. Using this formula, Connes' trace theorem is shown for operators of the form $M_f(1-\Delta)^{-\frac{d}{2}}$ on $L_2(\mathbb{R}^d)$, where M_f is multiplication by a function belonging to the Sobolev space $W_1^d(\mathbb{R}^d)$---the space of all integrable functions on $\mathbb{R}^d$ whose weak derivatives up to order d are all also integrable---and Δ is the Laplacian on $L_2(\mathbb{R}^d)$. An analogous formula for the Moyal plane is also shown.

The ζ-residue formula we derive also enables a second result. We consider the smoothed Riesz map g of the massless Dirac operator $\mathcal{D}$ on $\mathbb{R}^d$, for $d\geq 2$, and study its properties in terms of weak Schatten classes. Our sharp estimates, which are optimal in the scale of weak Schatten classes, show that the decay of singular values of $\mathrm{g}(\mathcal{D}+V)-\mathrm{g}(\mathcal{D})$ differs dramatically for the case when the perturbation V is a purely electric potential and the case when V is a magnetic one. The application of double operator integrals also yields a similar result for the operator $f(\mathcal{D}+V)-f(\mathcal{D})$ for an arbitrary monotone function f on $\mathbb{R}$ whose derivative is Schwartz.

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Abstract

This thesis is concerned first with a non-compact variation of Connes' trace theorem, which demonstrated that the Dixmier trace extends the notion of Lebesgue integration on a compact manifold. To obtain the variation, we develop a new ζ-residue formula, which is proved by an innovative approach using double operator integrals. Using this formula, Connes' trace theorem is shown for operators of the form $M_f(1-\Delta)^{-\frac{d}{2}}$ on $L_2(\mathbb{R}^d)$, where M_f is multiplication by a function belonging to the Sobolev space $W_1^d(\mathbb{R}^d)$—the space of all integrable functions on $\mathbb{R}^d$ whose weak derivatives up to order d are all also integrable—and Δ is the Laplacian on $L_2(\mathbb{R}^d)$. An analogous formula for the Moyal plane is also shown.

The ζ-residue formula we derive also enables a second result. We consider the smoothed Riesz map g of the massless Dirac operator $\mathcal{D}$ on $\mathbb{R}^d$, for $d \geq 2$, and study its properties in terms of weak Schatten classes. Our sharp estimates, which are optimal in the scale of weak Schatten classes, show that the decay of singular values of $\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})$ differs dramatically for the case when the perturbation V is a purely electric potential and the case when V is a magnetic one. The application of double operator integrals also yields a similar result for the operator $f(\mathcal{D}+V) - f(\mathcal{D})$ for an arbitrary monotone function f on $\mathbb{R}$ whose derivative is Schwartz.

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At some point near the end of 2016, a starry-eyed student with a fresh bachelor's degree in mathematics and a mind to pursue a PhD in mathematical physics visited Alan Carey at ANU. At that meeting, Alan advised the student that the prolific academic and his close collaborator, Fedor Sukochev, was likely a good person to speak to. Though not a mathematical physicist, Fedor's research in noncommutative geometry had inextricable roots in the area. Moreover, he worked at UNSW, the university where the student had conducted his undergrad studies. Within days, Fedor found the naïve stranger of a student knocking at his office door and (quite uncharacteristically, I might add) decided to accept him as a student almost immediately! I know not by what rubric he made that remarkable decision, but it was due to that decision—and Alan's direction—that the student was able to eventually produce the present thesis.

Fedor's supervision was as unconventional as it was effective. His broad insights, wisdom and perfectionism were all inspiring to behold and were a constant driver for the direction of my research, but balancing his own research projects with all of his research students, of which there were both numerous, was a nontrivial task. For this reason, I benefitted from the co-supervision of correspondingly numerous academics, each of whom were tasked with fostering a certain set of skills. Dima's door was always open, and he was constantly brimming with keen mathematical insights. He encouraged the pursuit of beauty and generality in results proven through clever argumentation. Steven countered this by ensuring my approach to mathematics remained grounded, rigorous, clearly written and timely, with his careful and time-consuming reading of my work time and time again resulting in essential course-correction. Meanwhile, Galina provided a balanced combination of the previous two approaches, and her fresh experience as a PhD student herself lent her a much-needed level of empathy and understanding. This thesis is the product of the joint supervision of these four, and my gratitude for their hard efforts and enduring patience is profound.

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Contents

1

Introduction

This thesis studies the spectral asymptotic properties of certain classical compact operators on $L_2(\mathbb{R}^d)$ associated to commutative and noncommutative Euclidean space. Namely, we study the spectral asymptotics of operators of the form $M_f(1-\Delta)^{-\frac{d}{2}}$, for Sobolev functions $f \in W_1^d(\mathbb{R}^d)$ (and its noncommutative analogue), where Δ denotes the Laplacian on $\mathbb{R}^d$, and $\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})$, where g is a smoothed Riesz map, $\mathcal{D}$ is the massless Dirac operator on $\mathbb{R}^d$ and V is a bounded electromagnetic potential.

1.1 Main results

A singular trace on a complete symmetric ideal $\mathcal{I}$ of $\mathcal{B}(\mathcal{H})$, where $\mathcal{H}$ is a separable Hilbert space, is a unitarily invariant linear functional which vanishes on the subspace of finite-rank operators in $\mathcal{I}$ [57]. In 1966, J. Dixmier [31] constructed an explicit example of a singular trace, now named the Dixmier trace, on the dual of the Macaev ideal, $\mathcal{M}_{1,\infty}$, which is defined by

$$\mathcal{M}_{1,\infty} := \Big\{ A \in \mathcal{K}(\mathcal{H}) \, : \, \sum_{j=0}^{n} \mu(j, A) = \mathcal{O}\big(\log(2+n)\big) \text{ as } n \uparrow \infty \Big\},$$

where $\big\{\mu(n, A)\big\}_{n=0}^{\infty}$ is the singular value sequence of the compact operator $A \in \mathcal{K}(\mathcal{H})$. The Dixmier trace is given by the expression

$$\mathrm{Tr}_\omega(A) = \omega\Big(\Big\{ \frac{1}{\log(2+j)} \sum_{k=0}^{j} \mu(k, A) \Big\}_{j \geq 0}\Big), \quad 0 \leq A \in \mathcal{M}_{1,\infty},$$

where ω is an extended limit on $\ell_\infty(\mathbb{N})$ (see Section 2.4.2 below for the details). In [31] (see also [24, §IV.2.β]), it is required that ω be invariant for the dilation semigroup on $\ell_\infty(\mathbb{N})$ for Tr_ω to be additive on $\mathcal{M}_{1,\infty}$. On the sub-ideal $\mathcal{L}_{1,\infty} \subset \mathcal{M}_{1,\infty}$, where

$$\mathcal{L}_{p,\infty} := \Big\{ A \in \mathcal{K}(\mathcal{H}) \, : \, \mu(n, A) = \mathcal{O}\Big(\frac{1}{(1+n)^p}\Big) \text{ as } n \uparrow \infty \Big\}, \quad 1 \leq p < \infty,$$

denote the weak Schatten classes, this dilation-invariance is, in fact, unnecessary [57, §9.7].

An operator $A \in \mathcal{M}_{1,\infty}$ is said to be Dixmier measurable if its Dixmier trace is independent of the choice of dilation-invariant extended limit ω. It is known that there exist Dixmier non-measurable operators in $\mathcal{L}_{1,\infty}$ [48, Theorem 1.4].

We now state the first main result of this thesis, which I showed with co-authors in [68].

Theorem 1.1. *Let* $0 \leq A, B \in \mathcal{B}(\mathcal{H})$ *such that* $[A^{\frac{1}{2}}, B] \in \mathcal{L}_1$. *Let* $C_{AB} \in \mathbb{R}$.

(*a*) *If* $AB \in \mathcal{M}_{1,\infty}$, *then the following are equivalent:*

- (*i*) AB *is Dixmier measurable, and* $\mathrm{Tr}_\omega(AB) = C_{AB}$ *for all dilation-invariant extended limits* ω.
- (*ii*) $\lim_{p\downarrow 1}(p-1)\,\mathrm{Tr}(B^p A^p) = C_{AB}$.

(*b*) *If* $AB \in \mathcal{L}_{1,\infty}$, *then part* (*a*) *also holds for any extended limit* ω.

Using this result, we study sharp Lipschitz-type estimates for the free (massless) Dirac operator on $\mathbb{R}^d$, which leads us to our second main result. Suppose $d \geq 2$ and let $N_d = 2^{\lfloor \frac{d}{2} \rfloor}$. Consider the Hilbert space $\mathbb{C}^{N_d} \otimes L_2(\mathbb{R}^d)$, and denote by γ_j, for $j = 1, \ldots, d$, the d-dimensional ($N_d \times N_d$) gamma matrices (see Section 2.2.2 below). Let

$$\mathcal{D} = \sum_{j=1}^{d} \gamma_j \otimes \frac{\partial}{i\,\partial t_j}$$

denote the free Dirac operator on $\mathbb{C}^{N_d} \otimes L_2(\mathbb{R}^d)$. We fix functions $\phi \in L_\infty(\mathbb{R}^d, \mathbb{R})$ (the *electric* or *scalar potential function*) and $\mathbf{A} = (a_1, \ldots, a_d) \in L_\infty(\mathbb{R}^d, \mathbb{R})^d$ (the *magnetic* or *vector potential function*), and consider the bounded, self-adjoint operator

$$V = \mathbb{I} \otimes M_\phi - \sum_{j=1}^{d} \gamma_j \otimes M_{a_j} \in \mathcal{B}\big(\mathbb{C}^{N_d} \otimes L_2(\mathbb{R}^d)\big), \tag{1.1}$$

where $\mathbb{I}$ denotes the $N_d \times N_d$ identity matrix, and M_f denotes the multiplication operator on $L_2(\mathbb{R}^d)$ by the function f.

I showed the second main result of this thesis with co-authors in [52]. This result gives the smallest ideal on the scale of weak Schatten ideals containing the operator $f(\mathcal{D}+V) - f(\mathcal{D})$ on $\mathbb{C}^{N_d} \otimes L_2(\mathbb{R}^d)$, where f is a real-valued function on $\mathbb{R}$ with finite distinct limits at $\pm\infty$ and derivative belonging to Schwartz space. We observe that when the vector potential $\mathbf{A} = 0$, the difference $f(\mathcal{D}+V) - f(\mathcal{D})$ exhibits radically different behaviour to the case when $\mathbf{A} \neq 0$. This is a consequence of the fact that the perturbation V does not have bounded commutator with $\mathcal{D}$ when $\mathbf{A} \neq 0$.

In the following, for $n \in \mathbb{N}$ and $1 \le p \le \infty$, the symbol $W_p^n(\mathbb{R}^d)$ denotes the Sobolev space of functions in $L_p(\mathbb{R}^d)$ whose weak derivatives up to order n are also L_p, and $\mathcal{S}(\mathbb{R}^d)$ denotes Schwartz space. If $\mathcal{I}$ is a complete symmetric ideal of $\mathcal{B}(\mathcal{H})$, let $\mathcal{I}_0$ denote the separable part of $\mathcal{I}$; that is, the closure of the subspace of finite-rank operators in $\mathcal{I}$.

Theorem 1.2. *Suppose $\phi \in (W^5_{\frac{d}{2}} \cap W^5_\infty)(\mathbb{R}^d)$ and $\mathbf{A} \in (W^2_{\frac{d}{2}} \cap W^2_\infty)(\mathbb{R}^d)^d$ are real-valued. Suppose $f : \mathbb{R} \to \mathbb{R}$ is a function such that $f' \in \mathcal{S}(\mathbb{R})$ and $f(-\infty) \neq f(+\infty)$.*

(i) If $\mathbf{A} = 0$ and $\phi \neq 0$, then $f(\mathcal{D}+V) - f(\mathcal{D}) \in \mathcal{L}_{\frac{d}{2},\infty} \setminus (\mathcal{L}_{\frac{d}{2},\infty})_0$.

(ii) If $\mathbf{A} \neq 0$, then $f(\mathcal{D}+V) - f(\mathcal{D}) \in \mathcal{L}_{d,\infty} \setminus (\mathcal{L}_{d,\infty})_0$.

These differences and their asymptotics are relevant for perturbation theory [91, §8.3].

1.2 Background and significance

1.2.1 The Dixmier trace and zeta residues

In 1988, in work which recovered the Yang–Mills action functional within the machinery of noncommutative geometry, A. Connes [23] demonstrated that the Dixmier trace is a linear extension of the Wodzicki residue. The residue Res_W is a trace defined on classical pseudo-differential operators of order $-d$ acting on sections of a complex vector bundle of a compact Riemannian manifold (see also [46], [24, §IV.2.β], [43, §7.3]).

We state below the more recent version of Connes' trace theorem given in [48, Corollary 7.22].

Theorem 1.3 (Connes trace theorem)**.** *Suppose M is a compact d-dimensional Riemannian manifold, and $B : C^\infty(M) \to C^\infty(M)$ is a classical pseudo-differential operator of order $-d$ with Wodzicki residue $\mathrm{Res}_W(B)$, then (the bounded extension of) B acting on $L_2(M)$ belongs to $\mathcal{L}_{1,\infty}$ and, for any extended limit ω, we have the equality*

$$\mathrm{Tr}_\omega(B) = \frac{1}{d(2\pi)^d}\,\mathrm{Res}_W(B).$$

This surprising result bespeaks a deep relationship between the asymptotic behaviour of the singular value sequence and the principal symbol of a pseudo-differential operator. It follows that the Dixmier trace is an extension of the notion of Lebesgue integration of L_2-functions on compact manifolds (see, e.g., [55, Theorem 2.5], [48, Theorem 1.5]):

Theorem 1.4 (Connes integration formula)**.** *Suppose M is a d-dimensional compact oriented Riemannian manifold without boundary. If $f \in L_2(M)$, then $M_f(1+\Delta)^{-\frac{d}{2}}$ belongs* *to* $\mathcal{L}_{1,\infty}$*, and there exists a constant* $C > 0$ *such that, for every extended limit* ω *on* $\ell_\infty(\mathbb{N})$*,*

$$\mathrm{Tr}_\omega\left(M_f(1+\Delta)^{-\frac{d}{2}}\right) = C \cdot \int_M f\,|\mathrm{dVol}_g|,$$

where M_f *denotes the multiplication operator on* $L_2(M)$ *for* f*, and* Δ *denotes the Hodge Laplacian on* M*.*

M. Wodzicki [90] showed that if B is a positive classical pseudo-differential operator of order $-d$, then the zeta function $\zeta_B(z) \coloneqq \mathrm{Tr}(B^z)$, for $\mathfrak{Re}(z) > 1$, has a meromorphic extension with simple poles, and $\mathrm{Res}_W(B)$ is proportional to the residue of the pole at $z = 1$. Connes [24] later highlighted that this residue property (at least when the residue is considered only as a right-hand limit on the real line) is also a general feature of the Dixmier trace, in that there is a connection between Dixmier measurability and the residue of the ζ-function at its leading singularity using the Karamata theorem [47]. We state a more recent refinement of this result given in [56, Corollary 6.8] (see also [57, Theorem 9.3.1]).

Theorem 1.5. *Suppose* $0 \le B \in \mathcal{M}_{1,\infty}$ *and* $0 \le C \in \mathbb{R}$*. The following are equivalent:*

- (i) *B is Dixmier measurable, and* $\mathrm{Tr}_\omega(B) = C$ *for all dilation-invariant extended limits* ω*.*
- (ii) $\lim_{\varepsilon\downarrow 0} \varepsilon\,\mathrm{Tr}(B^{1+\varepsilon}) = C$, *where* Tr *denotes the standard trace.*

Following a succession of results [20, Theorem 3.8], [22, Theorem 4.11], [56, Theorem 6.6], [85, Corollary 16], in 2017, the above theorem was generalised in [84], where it was shown that a variant of Theorem 1.5 continues to hold for non-positive operators in $\mathcal{L}_{1,\infty}$.

Theorem 1.6. [84, Theorem 1.2] *Suppose* $A \in \mathcal{B}(\mathcal{H})$*,* $0 \le B \in \mathcal{L}_{1,\infty}$ *and* $C \in \mathbb{C}$*. The following are equivalent:*

- (i) *AB is Dixmier measurable, and* $\mathrm{Tr}_\omega(AB) = C$ *for all dilation-invariant extended limits* ω*.*
- (ii) $\lim_{\varepsilon\downarrow 0} \varepsilon\,\mathrm{Tr}(AB^{1+\varepsilon}) = C$*.*

This emulates the noncommutative residue formula for $\mathbb{R}^d$; that is, when M is a compact d-dimensional Riemannian manifold, if $B \in \mathcal{B}\big(L_2(M)\big)$ is a classical order $-d$ pseudo-differential operator, one has [38, Theorem 1.7.7]

$$\mathrm{Res}_W(B) = d(2\pi)^d \lim_{\varepsilon\downarrow 0} \varepsilon\,\mathrm{Tr}\left(B_0(1+\Delta)^{-\frac{d(1+\varepsilon)}{2}}\right),$$

where Δ denotes the Hodge Laplacian on M and where $B_0 = B(1+\Delta)^{\frac{d}{2}}$ is an order 0 pseudo-differential operator.

The previous results require that $B \in \mathcal{K}(\mathcal{H})$. However, it can occur that both A and B are non-compact operators, but their product AB belongs to $\mathcal{L}_{1,\infty}$. For example, if $f \in \mathcal{S}(\mathbb{R}^d)$ is a nonzero Schwartz function and $\Delta = \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2}$ denotes the Laplacian on $L_2(\mathbb{R}^d)$, then neither the multiplication operator of f on $L_2(\mathbb{R}^d)$, denoted M_f, nor the resolvent $(1-\Delta)^{-\frac{d}{2}}$ acting on $L_2(\mathbb{R}^d)$ are compact operators, but their product $M_f(1-\Delta)^{-\frac{d}{2}}$ resides in $\mathcal{L}_{1,\infty}$ [7, 48]. There are analogous results to Theorems 1.5 and 1.6 in this case.

In 2012, A. Carey, V. Gayral, A. Rennie and F. Sukochev [16] established necessary conditions which we state below for the special case where the underlying semifinite von Neumann algebra is $\mathcal{B}(\mathcal{H})$. Note that an extended limit on $\ell_\infty(\mathbb{N})$ is called exponentiation-invariant if it is invariant for the exponentiation semigroup on $\ell_\infty(\mathbb{N})$.

Theorem 1.7. [16, Theorem 4.13] *Suppose* $0 \le A, B \in \mathcal{B}(\mathcal{H})$. *If there exists some* $\varepsilon > 0$ *such that* $[A^{\frac{1}{2}-\varepsilon}, B] \in (\mathcal{M}_{1,\infty})_0$ *and*

$$\sup_{1\le p\le 2} (p-1)\operatorname{Tr}(A^{\frac{1}{2}-\varepsilon} B^p A^{\frac{1}{2}-\varepsilon}) < \infty, \tag{1.2}$$

then $AB \in \mathcal{M}_{1,\infty}$ *and, if* $\lim_{p\downarrow 1}(p-1)\operatorname{Tr}(A^{\frac{1}{2}} B^p A^{\frac{1}{2}})$ *exists, then for any dilation- and exponentiation-invariant extended limit* ω,

$$\operatorname{Tr}_\omega(AB) = \lim_{p\downarrow 1}(p-1)\operatorname{Tr}(A^{\frac{1}{2}} B^p A^{\frac{1}{2}}). \tag{1.3}$$

Theorem 1.1 is an improvement of this result. Indeed, in Theorem 1.1, the requirement of exponentiation-invariant extended limits ω is dropped, thus yielding Dixmier measurability. Moreover, the conditions in Theorem 1.1 are easier to check in applications, as shown in Sections 3.3 and 3.4 below. We demonstrate this by applying Theorem 1.1 to two concrete examples of non-compact manifolds; one commutative and one noncommutative.

In Section 3.3, we confirm the assumption required in Theorem 1.1; that is,

$$\left[M_{f^{\frac{1}{2}}}, (1-\Delta)^{-\frac{d}{2}}\right] \in \mathcal{L}_1,$$

holds when $0 \le f \in \mathcal{S}(\mathbb{R}^d)$. We may then apply Theorem 1.1 to the pseudo-differential operators $M_f(1-\Delta)^{-\frac{d}{2}}$ on $\mathbb{R}^d$, with $A = M_f$ and $B = (1-\Delta)^{-\frac{d}{2}}$, and recover the classical formula

$$\operatorname{Tr}_\omega\left(M_f(1-\Delta)^{-\frac{d}{2}}\right) = \frac{\operatorname{Vol}(\mathbb{S}^{d-1})}{d(2\pi)^d}\int_{\mathbb{R}^d} f(\mathbf{x})\,\mathrm{d}\mathbf{x},$$

for Sobolev functions $f \in W_1^d(\mathbb{R}^d)$, where $\operatorname{Vol}(\mathbb{S}^{d-1})$ denotes the volume of the unit sphere $\mathbb{S}^{d-1}$ (see, e.g., [73, Corollary 14]).

We also use Theorem 1.1 to recover the analogous result for the noncommutative Euclidean (or Moyal) plane recently shown in [86, Theorem 1.1], where a different method was used.

Suppose the convolution of functions on $\mathbb{R}^2$ is 'twisted' by a real skew-symmetric matrix Θ. That is, for $f, g \in \mathcal{S}(\mathbb{R}^2)$, define $\diamond_\Theta$ by

$$(f \diamond_\Theta g)(\mathbf{t}) := \int_{\mathbb{R}^2} f(\mathbf{t})g(\mathbf{s}-\mathbf{t})e^{i\mathbf{t}\cdot\Theta\mathbf{s}}\,\mathrm{d}\mathbf{t}, \quad \mathbf{t} \in \mathbb{R}^2, \tag{1.4}$$

where $\Theta := \begin{pmatrix} 0 & \theta \\ -\theta & 0 \end{pmatrix}$, $\theta > 0$. This operation is the Fourier dual of the so-called Moyal product as studied in [74, 41, 42, 35].

Let $\mathrm{Op}_\Theta(f)$ correspond to left $\diamond_\Theta$-multiplication by a Schwartz function $f \in \mathcal{S}(\mathbb{R}^2)$; this provides an action of $\mathcal{S}(\mathbb{R}^2)$ onto itself which may be extended to a bounded linear operator on $L_2(\mathbb{R}^2)$ [53, Lemma 6.9]. In Section 3.4.3, we verify the condition required for Theorem 1.1 for those $f \in \mathcal{S}(\mathbb{R}^2)$ admitting $\mathrm{Op}_\Theta(f) \geq 0$; that is, the commutator

$$\left[\mathrm{Op}_\Theta(f)^{\frac{1}{2}}, (1-\Delta_\Theta)^{-1}\right] \in \mathcal{L}_1,$$

where the Laplace-type operator Δ_Θ is defined as in [53] by

$$\Delta_\Theta f(\mathbf{x}) = |\mathbf{x}|^2 f(\mathbf{x}), \quad f \in L_2^2(\mathbb{R}^2),\ \mathbf{x} \in \mathbb{R}^2,$$

where $L_2^2(\mathbb{R}^2)$ denotes a Bessel-weighted L_2-space (see Section 3.4.1 below).

For those Schwartz functions $f \in \mathcal{S}(\mathbb{R}^2)$ such that the operator $\mathrm{Op}_\Theta(f)$ is positive, we may appeal to Theorem 1.1 with $A = \mathrm{Op}_\Theta(f)$ and $B = (1-\Delta_\Theta)^{-1}$ to obtain the expression

$$\mathrm{Tr}_\omega\left(\mathrm{Op}_\Theta(f)(1-\Delta_\Theta)^{-1}\right) = \pi f(\mathbf{0}),$$

which agrees with [86, Proposition 4.5] (see Proposition 3.45 below). The Moyal algebra has an analogous construction of Sobolev elements, and we extend the result to these elements (as in [86]) by using noncommutative Cwikel estimates [53].

1.2.2 The smoothed signum and Lipschitz-type estimates

Let $\mathrm{g} \in C^\infty(\mathbb{R})$ denote the algebraic sigmoid function defined by the expression

$$\mathrm{g}(t) := \frac{t}{\sqrt{1+t^2}}, \quad t \in \mathbb{R}.$$

We call g the *smoothed signum* on $\mathbb{R}$. The continuity properties of g of the form

$$\left\|\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})\right\|_\infty \leq \mathrm{const} \cdot \|V\|_\infty$$

have important applications in the study of spectral flow, which was initiated by M. Atiyah and I. Singer in [4] and then connected to index theory in [2, 3]. Recently, the continuity of g for the case studied by Atiyah–Singer (the Dirac operator for perturbation of complete metrics on a smooth manifold) appears in [5].

It was conjectured by I. Singer [80] that, in the case of certain differential operators, spectral flow can be expressed as an integral of one forms. This idea received proper attention in [19], where spectral flow formulae using integrals of one forms were obtained. To work with analytic formulae for spectral flow for unbounded operators, one is forced to consider Schatten class estimates of the form

$$\big\|\mathrm{g}(\mathcal{D}+V)-\mathrm{g}(\mathcal{D})\big\|_p \leq \mathrm{const}\cdot\big\|V(1+\mathcal{D}^2)^{-\frac{1}{2}}\big\|_p, \tag{1.5}$$

where $\|\cdot\|_p$ denotes the norm on the Schatten ideal $\mathcal{L}_p$, $p\geq 1$. These types of operator estimates were studied extensively (see, e.g., [81] and references therein). Using the technique of double operator integrals, D. Potapov and F. Sukochev [66] obtained estimates (1.5) in their full generality, and then, together with A. Carey in [21] proved general integral formulae for spectral flow. Motivated by the study of the spectral shift function and the Fredholm/Witten index [36, 18], trace-class Lipschitz estimates of the form (1.5) were obtained for $d=1$.

Theorem 1.8. [17, Lemma 3.1] *If $f\in(W_1^1\cap C_{\mathrm{b}}^0)(\mathbb{R})$, then*

$$\mathrm{g}\Big(\frac{\mathrm{d}}{i\,\mathrm{d}x}+M_f\Big)-\mathrm{g}\Big(\frac{\mathrm{d}}{i\,\mathrm{d}x}\Big)\in\mathcal{L}_1\big(L_2(\mathbb{R})\big).$$

This trace-class result is not preserved in higher dimensions. We use Theorem 1.1, to obtain the higher-dimensional analogue for the free Dirac operator $\mathcal{D}$ on the Hilbert space $\mathbb{C}^{N_d}\otimes L_2(\mathbb{R}^d)$. As above, let $(\mathcal{L}_{p,\infty})_0$ be the closure of the subspace of all finite-rank operators in the quasi-norm

$$\|A\|_{p,\infty}\coloneqq\sup_{j\geq 0}(1+j)^{-\frac{1}{p}}\mu(j,A),\quad A\in\mathcal{L}_{p,\infty}.$$

Theorem 1.9. *Let $d\geq 2$, and suppose $\phi\in(W_{\frac{d}{2}}^5\cap W_\infty^5)(\mathbb{R}^d)$ and $\mathbf{A}\in(W_{\frac{d}{2}}^2\cap W_\infty^2)(\mathbb{R}^d)^d$ take values in $\mathbb{R}$ and $\mathbb{R}^d$, respectively. Let V be the self-adjoint operator in* (1.1) *above.*

(*i*) *If $\mathbf{A}=0$ and $\phi\neq 0$, then $\mathrm{g}(\mathcal{D}+V)-\mathrm{g}(\mathcal{D})\in\mathcal{L}_{\frac{d}{2},\infty}\setminus(\mathcal{L}_{\frac{d}{2},\infty})_0$.*

(*ii*) *If $\mathbf{A}\neq 0$, then $\mathrm{g}(\mathcal{D}+V)-\mathrm{g}(\mathcal{D})\in\mathcal{L}_{d,\infty}\setminus(\mathcal{L}_{d,\infty})_0$.*

By an argument relying on the double operator integral techniques initiated by M. Birman and M. Solomyak (see, e.g., [13]) and improved by D. Potapov and F. Sukochev (see

[65, 66]), we observe that the behaviour of singular values of $f(\mathcal{D}+V) - f(\mathcal{D})$, with $f' \in \mathcal{S}(\mathbb{R})$ and distinct limits at infinity, is the same as that of $\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})$. Hence, Theorem 1.2 follows from the above.

We sketch the idea for the proof of Theorem 1.9. One can represent the operator $\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})$ as the $\mathcal{K}(\mathcal{H})$-valued Bochner integral

$$\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) = \frac{1}{\pi}\,\Re\mathfrak{e}\left(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\Big(\frac{1}{\mathcal{D}+V+i(1+\lambda)^{\frac{1}{2}}} - \frac{1}{\mathcal{D}+i(1+\lambda)^{\frac{1}{2}}}\Big)\right),$$

which facilitates its decomposition into the form

$$\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) \in \sum_\alpha M_{\mathrm{F}_\alpha}\big(\mathbb{I}\otimes g_\alpha(\nabla)\big) + \mathcal{L}_p,$$

where F_α is some bounded (hermitian) matrix-valued function on $\mathbb{R}^d$, g_α is a bounded real-valued on $\mathbb{R}^d$, ∇ denotes the gradient operator, and where either $p = \frac{d}{2}$ if the magnetic part of V is zero, or $p = d$ otherwise. The inclusion $M_{\mathrm{F}_\alpha}\big(\mathbb{I}\otimes g_\alpha(\nabla)\big) \in \mathcal{L}_{p,\infty}$ in each case is shown using Cwikel estimates [27, 7].

To prove sharpness, recall that if an operator A belongs to $(\mathcal{L}_{p,\infty})_0$, then it follows from the Hölder inequality [79] that if $B \in \mathcal{L}_{q,\infty}$, where $\frac{1}{p}+\frac{1}{q} = 1$, then $AB \in (\mathcal{L}_{1,\infty})_0$. It is shown using Theorem 1.1 that there exist $B \in \mathcal{L}_{q,\infty}$ such that

$$\mathrm{Tr}_\omega\big(\mathrm{g}(\mathcal{D}+V)B - \mathrm{g}(\mathcal{D})B\big) \neq 0,$$

so that $\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) \notin (\mathcal{L}_{p,\infty})_0$ by contradiction, since Tr_ω vanishes on $(\mathcal{L}_{1,\infty})_0$.

1.3 Structure of the thesis

Chapter 2 recalls preliminary material and the notational conventions employed in this thesis. In Section 2.2, we recall some of the fundamental properties of unbounded operators on Hilbert space, including weak derivatives on $L_2(\mathbb{R}^d)$, the classic Laplacian and the free Dirac operator on $\mathbb{R}^d$.

In Section 2.3, we recall two-sided ideals of compact operators, the Calkin correspondence, as well as the definitions and properties of (weak) Schatten classes and the Dixmier–Macaev ideal. We also recall the definition of a (symmetric) quasi-Banach ideal and the notion of a trace on such an ideal in Section 2.4. In particular, we recall the properties of the classical trace Tr on $\mathcal{L}_1$ in Section 2.4.1 and the Dixmier traces on $\mathcal{M}_{1,\infty}$ and $\mathcal{L}_{1,\infty}$ in Section 2.4.2, with examples of classical operators which belong to these ideals in Section 2.5. We introduce Cwikel estimates [10, 77, 27, 7] (Section 2.5.2) and double operator integration (Section 2.6.2), the latter of which is defined using the weak operator integral approach seen in [25] (see also Section 2.6.1).

Chapter 3 presents the contents of the paper [68], in which Theorem 1.1 is proven. In Section 3.1, a trace-class variant of [24, Lemma 11 (§IV.3.α)] (Proposition 3.3) is proven using the double operator integral techniques in [25, 87]. Some technical but elementary arguments in the proof of this result may be found in Appendix A.1. Theorem 1.1 then follows quickly from this result, as seen in Section 3.2 below. A special case of Connes' trace theorem (Theorem 3.16) on $\mathbb{R}^d$ is shown in Section 3.3.2 by demonstrating that the simple hypotheses of Theorem 1.1 hold for operators of the form $M_f(1-\Delta)^{-\frac{d}{2}}$, for $0 \leq f \in \mathcal{S}(\mathbb{R}^d)$ (we use the regularity properties of $f^{\frac{1}{2}}$ seen in Section 3.3.1); the result for general $f \in W_1^d(\mathbb{R}^d)$ is shown by a density argument. Similarly, it is shown in Section 3.4.3 that the trace theorem for the Moyal plane seen in [86] may be recovered using Theorem 1.1. To this end, the underlying matricial structure of noncommutative Schwartz space is essential, and is discussed in Section 3.4.2.

The contents of [52] are then given in Chapter 4, including the proofs of Theorems 1.2 and 1.9 above. A key Bochner integral decomposition and convenient versions of Cwikel estimates are written in Section 4.1.1. The electric and magnetic cases are split into two separate arguments (Sections 4.1.2 and 4.1.3, respectively), since the magnetic decomposition is significantly different from the electric case. Some Bochner integrals are computed explicitly in Appendix A.2. In Section 4.1.4, the sharp estimates of Theorem 1.9 are proven using the Cwikel estimates from Section 2.5.2 and a special case of Connes' trace theorem found in Section 3.3.2 (specifically, Lemma 3.15 therein). Double operator integral techniques are then employed in Section 4.2 to obtain Theorem 1.2.

List of publications

[**52**] G. Levitina, F. Sukochev, D. Vella and D. Zanin, “Schatten class estimates for the Riesz map of massless Dirac operators.” *Integral Equations Operator Theory* **90** (2018), no. 2, art. 19, 36 pp.

[**68**] D. Potapov, F. Sukochev, D. Vella and D. Zanin, “A residue formula for locally compact noncommutative manifolds.” **To appear** in *Positivity and Noncommutative Analysis: Festschrift in Honour of Ben de Pagter on the Occasion of his 65th Birthday* (2019).

Talks delivered during candidature

- 2017, *The Dirac operator and weak Schatten ideals*, School of Mathematics and Statistics Postgraduate Conference, UNSW, delivered 7 June 2017.
- 2018, *Dixmier traces in the noncommutative plane*, School of Mathematics and Statistics Postgraduate Conference, UNSW, delivered 8 June 2018.
- 2018, *The residue formula and Connes' trace theorem*, Analysis Seminar Series, UNSW, delivered 6 September 2018.

2

Preliminaries

2.1 Notations

In this section, we compile the notations used throughout the thesis.

The symbols $\mathbb{N}$, $\mathbb{Z}$, $\mathbb{R}$ and $\mathbb{C}$ denote the sets of all natural numbers, integers, real numbers and complex numbers, respectively. We adopt the convention $0 \in \mathbb{N}$, and we let $\mathbb{Z}_+ := \mathbb{N} \setminus \{0\}$. We also let $\mathbb{N}_\infty := \mathbb{N} \cup \{\infty\}$ denote the extended natural numbers.

The symbol $d \in \mathbb{Z}_+$ is usually used to refer to the dimension of a manifold, especially Euclidean space. The symbol m denotes the standard Lebesgue measure on $\mathbb{R}^d$, and the symbol $\#$ denotes the counting measure on $\mathbb{N}^d$ or $\mathbb{Z}^d$. $\mathbb{S}^{d-1}$ denotes the unit sphere in $\mathbb{R}^d$, and

$$\mathrm{Vol}(\mathbb{S}^{d-1}) = \frac{d\pi^{\frac{d}{2}}}{\Gamma(1+\frac{d}{2})}$$

denotes its geometric volume, where Γ denotes the Gamma function. If $\Omega \subset \mathbb{R}^d$ is an open region of the plane, then $\partial\Omega$ denotes its boundary.

If V is a topological vector space, we let V^* denote its topological dual space. Recall that a quasi-norm ρ on a (complex) vector space V is a non-negative real-valued function that is subadditive, (absolutely) homogeneous, and satisfies the following:

$$\text{there exists } C > 0 \text{ such that, for all } v, w \in V, \quad \rho(v+w) \leq C\big(\rho(v) + \rho(w)\big).$$

Recall also that, since every quasi-normed space is metrizable [6, Lemma 3.10.1], if V is a quasi-normed space which is complete with respect to its metric, then V is called a quasi-Banach space. If X is a generic Banach (or quasi-Banach) space, then we denote its corresponding norm (or quasi-norm) by $\|\cdot\|_X$. Moreover, we denote the inner product of a generic Hilbert space $\mathcal{H}$ by $\langle\cdot,\cdot\rangle$; the underlying Hilbert space corresponding to an inner product shall be clear from the context.

Let $0 < p < \infty$. If $\Omega \subset \mathbb{R}^d$ is a Lebesgue-measurable set, then we let $L_p(\Omega)$ denote the usual L_p-space on the measure space (Ω, m). For $1 \le p < \infty$, we denote the Banach norm on $L_p(\Omega)$ by $\|\cdot\|_p$. Moreover, we let $L_0(\Omega)$ denote the space of all Lebesgue-measurable functions on Ω, and $L_\infty(\Omega)$ denote the space of all essentially bounded functions on Ω (the Banach norm on the latter shall be denoted by $\|\cdot\|_\infty$). Additionally, for $1 \le p < \infty$, we let $L_{p,\infty}(\Omega)$ denote weak L_p-space on the measure space (Ω, m) equipped quasi-norm $\|\cdot\|_{p,\infty}$.

We also let $\ell_p(\mathbb{N}^d)$, $\ell_{p,\infty}(\mathbb{N}^d)$ (or $\ell_p(\mathbb{Z}^d)$, $\ell_{p,\infty}(\mathbb{Z}^d)$) denote the corresponding L_p- and weak L_p-spaces on the measure space $(\mathbb{N}^d, \#)$ (resp. $(\mathbb{Z}^d, \#)$). We denote their corresponding norms/quasi-norms by $\|\cdot\|_p$, $\|\cdot\|_{p,\infty}$, respectively. Note that, while the notation $\|\cdot\|_p$ denotes both the norm on $L_p(\Omega)$, for $\Omega \subset \mathbb{R}^d$, and the norms on $\ell_p(\mathbb{N}^d)$ and $\ell_p(\mathbb{Z}^d)$, the distinction between them shall be clear from context (the same applies to the notation $\|\cdot\|_{p,\infty}$).

We let $c_0(\mathbb{N})$, and $c_{00}(\mathbb{N})$, denote the spaces of sequences converging to zero, and eventually zero, respectively.

Suppose $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}^d$ is a multi-index. Let

$$|\boldsymbol{\alpha}| \coloneqq \alpha_1 + \dots + \alpha_d,$$

and let $\nabla^{\boldsymbol{\alpha}}$ be the mixed partial (distributional) differentiation operator given by

$$\nabla^{\boldsymbol{\alpha}} \coloneqq (-i)^{|\boldsymbol{\alpha}|} \frac{\partial^{\alpha_1}}{\partial x_k^{\alpha_1}} \cdots \frac{\partial^{\alpha_d}}{\partial x_k^{\alpha_d}}.$$

Suppose $0 \le s < \infty$ and $1 \le p \le \infty$. Let $W_p^s(\mathbb{R}^d)$ denote Bessel potential space. In particular, if $s \in \mathbb{N}$, this is equivalent to Sobolev space [44, §6.2], in which case we denote the Sobolev norm by

$$\|f\|_{W_p^s} \coloneqq \sum_{|\boldsymbol{\alpha}| \le s} \|\nabla^{\boldsymbol{\alpha}} f\|_p, \quad \text{for } f \in W_p^s(\mathbb{R}^d).$$

We let $L_{2,\mathrm{loc}}(\mathbb{R}^d)$ denote the space of all locally square-integrable functions on $\mathbb{R}^d$.

Suppose $n \in \mathbb{N}_\infty$. If $\Omega \subset \mathbb{R}^d$, we let $C^n(\Omega)$ denote the space of all C^n-functions on Ω; that is, continuous functions on Ω whose first n derivatives are also continuous. Additionally, we let $C^n_{\mathrm{b}}(\Omega)$ and $C^n_{\mathrm{com}}(\Omega)$ denote the subspaces of $C^n(\Omega)$ consisting of all bounded and compactly supported functions on Ω, respectively. We let $\mathcal{S}(\mathbb{R}^d)$ denote Schwartz space (the space of all rapidly decreasing smooth functions on $\mathbb{R}^d$), and let $\mathcal{F}$ denote the Fourier transform (both on $\mathcal{S}(\mathbb{R}^d)$ and its linear extension to $L_2(\mathbb{R}^d)$). To avoid ambiguity, we specify that $\mathcal{F}$ is considered in its unitary radial form:

$$(\mathcal{F}f)(\mathbf{x}) \coloneqq \frac{1}{(2\pi)^{\frac{d}{2}}} \int_{\mathbb{R}^d} f(\mathbf{t}) e^{-i\mathbf{x}\cdot\mathbf{t}} \, \mathrm{d}\mathbf{t}, \quad f \in \mathcal{S}(\mathbb{R}^d), \ \mathbf{x} \in \mathbb{R}^d.$$

For further details on weak L_p-spaces, Sobolev spaces, Schwartz space and the Fourier transform, the reader is referred to [44, 45].

If A is an operator on a Hilbert space $\mathcal{H}$, we let $\mathrm{dom}(A)$ denote its domain of definition, $\mathrm{ran}(A)$ denote its range, and $\sigma(A)$ denote its spectrum. If A is injective, then we denote its inverse operator by A^{-1}. We let $\mathcal{B}(\mathcal{H})$, $\mathcal{K}(\mathcal{H})$ and $\mathcal{C}_{00}(\mathcal{H})$ denote the spaces of all bounded, compact and finite-rank operators on $\mathcal{H}$, respectively. We let $\|\cdot\|_\infty$ denote the uniform norm on $\mathcal{B}(\mathcal{H})$.

Throughout this thesis, every Hilbert space $\mathcal{H}$ is assumed to be separable and infinite-dimensional.

We also define the special function $\langle\cdot\rangle : \mathbb{C}^d \to [1,\infty)$ by

$$\langle \mathbf{z} \rangle \coloneqq \big(1 + |\mathbf{z}|^2\big)^{\frac{1}{2}}, \quad \text{for } \mathbf{z} \in \mathbb{C}^d.$$

As a function on $\mathbb{R}^d$, it follows from the definition of weak L_p-space and the unboundedness of the harmonic series that

$$\langle\cdot\rangle^{-\frac{d}{p}} \in L_{p,\infty}(\mathbb{R}^d) \setminus L_p(\mathbb{R}^d).$$

Finally, if $\mathcal{I}(\mathcal{H}) \subset \mathcal{B}(\mathcal{H})$ is an ideal of $\mathcal{B}(\mathcal{H})$ and $A \in \mathcal{B}(\mathcal{H})$, then we denote the *coset* of A with respect to the ideal $\mathcal{I}(\mathcal{H})$ by

$$A + \mathcal{I}(\mathcal{H}) \coloneqq \big\{A + B \in \mathcal{B}(\mathcal{H}) \,:\, B \in \mathcal{I}(\mathcal{H})\big\}.$$

That is, if $B \in \mathcal{B}(\mathcal{H})$ and there exists some $B_0 \in \mathcal{I}(\mathcal{H})$ such that $B = A + B_0$, then one may write that $B \in A + \mathcal{I}(\mathcal{H})$. In our notations, we may suppress dependence upon the underlying Hilbert space $\mathcal{H}$, and simply write $\mathcal{I} = \mathcal{I}(\mathcal{H})$.

2.2 Unbounded operators

Suppose $\mathcal{H}$ is a Hilbert space, and let $A : \mathrm{dom}(A) \to \mathcal{H}$ be a densely-defined (linear) operator on $\mathcal{H}$. Let

$$\mathrm{dom}(A^*) \coloneqq \big\{g \in \mathcal{H} \,:\, \exists g' \in \mathcal{H} \text{ s.t. } \langle Af, g\rangle = \langle f, g'\rangle, \forall f \in \mathrm{dom}(A)\big\}.$$

By the Riesz representation theorem, for every $g \in \mathcal{H}$, the vector g' satisfying the equation $\langle Af, g\rangle = \langle f, g'\rangle$ is unique, and so we can define the *adjoint operator* of A, denoted A^*, by

$$A^* g \coloneqq g', \quad \text{for } g \in \mathrm{dom}(A^*),$$

If $\mathrm{dom}(A) = \mathrm{dom}(A^*)$, we denote the *real and imaginary parts* of A by

$$\mathfrak{Re}(A) \coloneqq \frac{1}{2}(A + A^*), \quad \mathfrak{Im}(A) \coloneqq \frac{1}{2i}(A - A^*).$$

If $\mathrm{dom}(A) \subseteq \mathrm{dom}(A^*)$ and $Af = A^*f$ for all $f \in \mathrm{dom}(A)$, then A is called a *symmetric operator*. If A is symmetric and $\mathrm{dom}(A) = \mathrm{dom}(A^*)$, then A is called a *self-adjoint operator*. If A is self-adjoint, then we let E_A denotes its projection-valued spectral measure (see, e.g., [69, §VIII.3]).

An operator $A : \mathrm{dom}(A) \to \mathcal{H}$ is said to be *positive* if

$$\langle Af, f\rangle_{\mathcal{H}} \geq 0, \qquad \text{for all } f \in \mathrm{dom}(A).$$

A is said to be *closed* if the graph of A,

$$\Gamma(A) := \big\{ f \oplus Af \in \mathcal{H} \oplus \mathcal{H} \,:\, f \in \mathrm{dom}(A) \big\},$$

is a closed subspace of $\mathcal{H} \oplus \mathcal{H}$. If A is closed, then we let $\mathrm{U}(A)$ denote its phase and $|A|$ denote its absolute value—$\mathrm{U}(A)$ is a partial isometry, $|A|$ is a positive self-adjoint operator, and their existence is guaranteed by the polar decomposition [69, Theorem VIII.32].

Suppose A, B are operators on the Hilbert space $\mathcal{H}$. We call B an *extension* of A if $\Gamma(A) \subseteq \Gamma(B)$ and $Af = Bf$, for all $f \in \mathrm{dom}(A)$.

An operator A is said to be *closable* if there exists a closed extension of A. If A is closable, then the closed extension of A with the smallest graph in $\mathcal{H} \oplus \mathcal{H}$ is called the *closure* of A. If A is closable with self-adjoint closure, then A is called *essentially self-adjoint*. If A is closed, a subset $X \subset \mathrm{dom}(A)$ is called a *core* for A if the closure of the restriction $A|_X$ is equal to A. In the sequel, we shall identify a closed operator A with any restrictions of A to its cores.

2.2.1 Commutators of operators

If A, B are operators on $\mathcal{H}$ with domains $\mathrm{dom}(A)$, $\mathrm{dom}(B)$, respectively, then we may define the operator AB on the domain

$$\mathrm{dom}(AB) := \big\{ f \in \mathrm{dom}(B) \,:\, Bf \in \mathrm{dom}(A) \big\}$$

by the expression

$$ABf := A(Bf), \quad f \in \mathrm{dom}(AB).$$

Definition 2.1. Suppose A is an operator on $\mathcal{H}$ with domain $\mathrm{dom}(A)$, and suppose $B \in \mathcal{B}(\mathcal{H})$ such that $B\big(\mathrm{dom}(A)\big) \subset \mathrm{dom}(A)$. The *commutator* of A and B is the operator $[A, B]$ with domain $\mathrm{dom}(A)$ defined by the expression

$$[A, B] := AB - BA.$$

The commutator satisfies the following algebraic properties, which we shall use in Chapter 4:

Lemma 2.2. *Suppose A is an operator on $\mathcal{H}$ with domain $\operatorname{dom}(A)$, and suppose B is a bounded operator on $\mathcal{H}$ such that $B\big(\operatorname{dom}(A)\big) \subset \operatorname{dom}(A)$.*

(*i*) *If $A : \operatorname{dom}(A) \to \mathcal{H}$ has bounded inverse, then the operator $[A^{-1}, B] : \mathcal{H} \to \mathcal{H}$ can be written as*

$$[A^{-1}, B] = -A^{-1}[A, B]A^{-1}, \tag{2.1}$$

where

$$A^{-1} : \mathcal{H} \to \operatorname{dom}(A), \quad A^{-1}[A, B] : \operatorname{dom}(A) \to \mathcal{H}.$$

(*ii*) *If $n \geq 1$, then the operator $[A, B^n] : \operatorname{dom}(A) \to \mathcal{H}$ can be decomposed as*

$$[A, B^n] = \sum_{k=0}^{n-1} B^k [A, B] B^{n-k-1} \tag{2.2}$$

on the domain $\operatorname{dom}(A)$.

Proof. (*i*): Since $B\big(\operatorname{dom}(A)\big) \subset \operatorname{dom}(A)$, we have that

$$ABA^{-1} : \mathcal{H} \overset{A^{-1}}{\to} \operatorname{dom}(A) \overset{B}{\to} \operatorname{dom}(A) \overset{A}{\to} \mathcal{H}$$

is well-defined on $\mathcal{H}$. Hence,

$$A^{-1}[A, B]A^{-1} = A^{-1}ABA^{-1} - A^{-1}BAA^{-1} = BA^{-1} - A^{-1}B = -[A^{-1}, B].$$

(*ii*). Since $B\big(\operatorname{dom}(A)\big) \subset \operatorname{dom}(A)$, we also have that $B^k\big(\operatorname{dom}(A)\big) \subset \operatorname{dom}(A)$, for all $k \in \mathbb{N}$, so the operators $B^k A B^{n-k}$ are well-defined on the domain $\operatorname{dom}(A)$, for all $k = 0, \ldots, n$. Hence,

$$[A, B^n] = AB^n - B^n A = \sum_{k=0}^{n-1} (B^k A B^{n-k} - B^{k+1} A B^{n-k-1}) = \sum_{k=0}^{n-1} B^k [A, B] B^{n-k-1}. \quad \square$$

2.2.2 Partial differentiation operators over $\mathbb{R}^d$

Recall that, for $n \in \mathbb{N}$ and $1 \leq p \leq \infty$, Sobolev space is denoted by $W_p^n(\mathbb{R}^d)$, and the Sobolev norm by $\|\cdot\|_{W_p^n}$.

Definition 2.3. For each $k = 1, \ldots, d$, we denote by ∂_k the kth *partial differentiation operator*, defined as

$$(\partial_k f)(\mathbf{x}) := -i \frac{\partial f}{\partial x_k}(\mathbf{x}), \quad \text{for } f \in C^\infty_{\text{com}}(\mathbb{R}^d),\ \mathbf{x} \in \mathbb{R}^d.$$

For each $k = 1, \ldots, d$, ∂_k is a essentially self-adjoint operator on $L_2(\mathbb{R}^d)$ whose closure is defined on the domain [76, Proposition 8.2]

$$\mathrm{dom}(\partial_k) := \Big\{ f \in L_2(\mathbb{R}^d) \ : \ \frac{\partial f}{\partial x_k} \in L_2(\mathbb{R}^d) \Big\}.$$

Hence, any subset of $\mathrm{dom}(\partial_k)$ containing $C^\infty_{\mathrm{com}}(\mathbb{R}^d)$ is a core for ∂_k (this includes Schwartz space $\mathcal{S}(\mathbb{R}^d)$ and Sobolev space $W^1_2(\mathbb{R}^d)$). Additionally, on $W^2_2(\mathbb{R}^d)$, we have that the commutator

$$[\partial_j, \partial_k] = 0, \quad j, k = 1, \ldots, d. \tag{2.3}$$

The reader is advised that the symbol ∂_k may also be used to refer to the distributional partial derivative of a vector from Sobolev spaces other than $W^1_2(\mathbb{R}^d)$; that is,

$$\partial_k f := -i \frac{\partial f}{\partial x_k} \in L_p(\mathbb{R}^d), \quad \text{for } f \in W^1_p(\mathbb{R}^d),\, 1 \leq p \leq \infty.$$

Definition 2.4. We denote by Δ the *Laplace operator* on $L_2(\mathbb{R}^d)$ with domain $W^2_2(\mathbb{R}^d)$ defined by the expression

$$\Delta := -\sum_{k=1}^d \partial_k^2, \quad \mathrm{dom}(\Delta) := W^2_2(\mathbb{R}^d).$$

The operator $-\Delta$ is positive and self-adjoint [76, Proposition 8.2].

The following definition of the Dirac operator over $\mathbb{R}^d$ is standard (see, e.g., [88, §8.5], [37, Chapter 4], [51, Chapter II]). Let $N_d := 2^{\lfloor \frac{d}{2} \rfloor}$, and we denote by $\mathbb{I} := \mathbb{I}_{N_d}$ the $N_d \times N_d$ identity matrix.

Definition 2.5. If $\{\gamma_j\}_{j=1}^d$ is a family of $N_d \times N_d$ matrices satisfying

$$(i)\ \gamma_j = \gamma_j^*,\ \gamma_j^2 = \mathbb{I},\ \text{for all } j = 1, \ldots, d;\ \text{and},$$
$$(ii)\ \gamma_j \gamma_k = -\gamma_k \gamma_j,\ \text{whenever } j \neq k,$$

we call $\{\gamma_j\}_{j=1}^d$ a family of *d-dimensional symmetric gamma matrices.*

Definition 2.6. The *(free) Dirac operator* on $\mathbb{C}^{N_d} \otimes L_2(\mathbb{R}^d)$ is an unbounded operator defined by

$$\mathcal{D} = \sum_{k=1}^d \gamma_k \otimes \partial_k, \qquad \mathrm{dom}(\mathcal{D}) = \mathbb{C}^{N_d} \otimes W^1_2(\mathbb{R}^d). \tag{2.4}$$

It is known that $\mathcal{D}$ is self-adjoint (essential self-adjointness follows from [69, Theorem VIII.33]; one can check closure by showing that the graph norm of $\mathcal{D}$ is equivalent to $\|\cdot\|_{\mathbb{C}^{N_d} \otimes W^1_2(\mathbb{R}^d)}$). Moreover, on the domain $\mathbb{C}^{N_d} \otimes W^2_2(\mathbb{R}^d)$,

$$\mathcal{D}^2 = \sum_{j,k=1}^d \gamma_j \gamma_k \otimes \partial_j \partial_k = \sum_{k=1}^d \mathbb{I} \otimes \partial_k^2 + \sum_{j>k} \gamma_j \gamma_k \otimes [\partial_j, \partial_k] \overset{(2.3)}{=} \mathbb{I} \otimes (-\Delta).$$

Definition 2.7. Suppose $f \in L_{2,\mathrm{loc}}(\mathbb{R}^d)$. We let M_f denote the *(pointwise) multiplication operator* of f, which is the operator on the Hilbert space $L_2(\mathbb{R}^d)$ defined by

$$(M_f g)(\mathbf{x}) \coloneqq f(\mathbf{x})g(\mathbf{x}), \quad g \in \mathrm{dom}(M_f),\ \mathbf{x} \in \mathbb{R}^d,$$

where

$$\mathrm{dom}(M_f) \coloneqq \big\{g \in L_2(\mathbb{R}^d) \,:\, f \cdot g \in L_2(\mathbb{R}^d)\big\}.$$

Note that if f is real-valued, then M_f is densely defined and self-adjoint [76, Example 3.8], and if $f \in L_\infty(\mathbb{R}^d)$, then $M_f \in \mathcal{B}\big(L_2(\mathbb{R}^d)\big)$. We observe the following identities:

Lemma 2.8. *Suppose $f \in W^1_\infty(\mathbb{R}^d)$, and let $k = 1, \dots, d$. Then the commutator $[\partial_k, M_f]$ extends to a bounded operator on $L_2(\mathbb{R}^d)$, and*

$$[\partial_k, M_f] = M_{\partial_k f}. \tag{2.5}$$

Proof. By the Leibniz rule [44, Proposition 2.3.22], $M_f g \in W^1_2(\mathbb{R}^d)$ for all $g \in C^\infty_{\mathrm{com}}(\mathbb{R}^d)$. Since $C^\infty_{\mathrm{com}}(\mathbb{R}^d)$ is dense in $W^1_2(\mathbb{R}^d)$, it follows from a standard density argument that

$$M_f\big(W^1_2(\mathbb{R}^d)\big) \subset W^1_2(\mathbb{R}^d).$$

Hence, it suffices to show that $[\partial_k, M_f]g = M_{\partial_k f}g$, for all $g \in \mathcal{S}(\mathbb{R}^d)$. If $g \in \mathcal{S}(\mathbb{R}^d)$, then by the Leibniz rule [44, Proposition 2.3.22], we have that

$$\partial_k(M_f g) = \partial_k(f \cdot g) = -i\frac{\partial(f \cdot g)}{\partial x_k} = -i\frac{\partial f}{\partial x_k} \cdot g - if \cdot \frac{\partial g}{\partial x_k} = M_{\partial_k f}g + M_f \partial_k g.$$

Rearranging this, one obtains the expression

$$[\partial_k, M_f]g = M_{\partial_k f}g, \quad \text{for all } g \in \mathcal{S}(\mathbb{R}^d). \qquad \square$$

Corollary 2.9. *For every $f \in W^1_\infty(\mathbb{R}^d)$, the commutator $[\mathcal{D}, \mathbb{I} \otimes M_f]$ extends to a bounded operator on $\mathbb{C}^{N_d} \otimes L_2(\mathbb{R}^d)$, and*

$$[\mathcal{D}, \mathbb{I} \otimes M_f] = \sum_{k=1}^d \gamma_k \otimes M_{\partial_k f}. \tag{2.6}$$

Proof. By Proposition 2.8, we have that

$$\begin{aligned}[\mathcal{D}, \mathbb{I} \otimes M_f] = \sum_{k=1}^d [\gamma_k \otimes \partial_k, \mathbb{I} \otimes M_f] &= \sum_{k=1}^d \big((\gamma_k \otimes \partial_k)(\mathbb{I} \otimes M_f) - (\mathbb{I} \otimes M_f)(\gamma_k \otimes \partial_k)\big) \\ &= \sum_{k=1}^d \gamma_k \otimes [\partial_k, M_f] \overset{(2.5)}{=} \sum_{k=1}^d \gamma_k \otimes M_{\partial_k f}\end{aligned}$$

over the domain $W^1_2(\mathbb{R}^d)^{N_d}$. $\square$

We state one more corollary that we shall use in Chapter 4 below. It immediately follows from the previous corollary and Lemma 2.2 (i).

Corollary 2.10. *Suppose $\lambda \in \mathbb{R} \setminus \{0\}$. For every $f \in W^1_\infty(\mathbb{R}^d)$, we have*

$$\big[(\mathcal{D}+i\lambda)^{-1}, \mathbb{I}\otimes M_f\big] = -\sum_{k=1}^{d}(\mathcal{D}+i\lambda)^{-1}(\gamma_k \otimes M_{\partial_k \phi})(\mathcal{D}+i\lambda)^{-1}. \tag{2.7}$$

2.3 Ideals of compact operators

For further details on two-sided ideals of $\mathcal{B}(\mathcal{H})$, the reader is referred to [40, 79]

Definition 2.11. A two-sided ideal $\mathcal{I}$ of $\mathcal{B}(\mathcal{H})$ is called a *Banach* (or a *quasi-Banach*) *ideal* if there exists a norm (resp. quasi-norm) $\|\cdot\|_{\mathcal{I}}$ on $\mathcal{I}$ satisfying the symmetric property,

$$\|ABC\|_{\mathcal{I}} \leq \|A\|_\infty \|B\|_{\mathcal{I}} \|C\|_\infty, \quad \text{for all } B \in \mathcal{I}(\mathcal{H}), \text{ and } A, C \in \mathcal{B}(\mathcal{H}),$$

such that $\big(\mathcal{I}, \|\cdot\|_{\mathcal{I}}\big)$ is a Banach (resp. quasi-Banach) space.

In general, it is not necessarily true that a sum belonging to $\mathcal{I}$ is a sum of operators each belonging to $\mathcal{I}$. However, one may exploit the properties of the gamma matrices (recall Definition 2.5 above) to obtain the following technical result, which we shall depend upon in Section 4.1.4 below.

Lemma 2.12. *Let $\mathcal{H}$ be a (separable) Hilbert space, and suppose $\mathcal{I}$ is an ideal of $\mathcal{B}(\mathcal{H})$.*

(i) *If $A_j \in \mathcal{B}(\mathcal{H})$, for $j = 1, \dots, d$, and*

$$\sum_{j=1}^{d} \gamma_j \otimes A_j \in \mathcal{I}(\mathbb{C}^{N_d} \otimes \mathcal{H}),$$

then $A_j \in \mathcal{I}(\mathcal{H})$, for every $j = 1, \dots, d$.

(ii) *If $B_{j,k} \in \mathcal{B}(\mathcal{H})$, for $j, k = 1, \dots, d$ with $j < k$, and*

$$\sum_{j<k} \gamma_j \gamma_k \otimes B_{j,k} \in \mathcal{I}(\mathbb{C}^{N_d} \otimes \mathcal{H}),$$

then $B_{j,k} \in \mathcal{I}(\mathcal{H})$, for every $j, k = 1, \dots, d$ with $j < k$.

Proof. (i). Fix any $k = 1, \dots, d$. For brevity, let $\mathcal{A} \in \mathcal{B}(\mathbb{C}^{N_d} \otimes \mathcal{H})$ be the operator given by

$$\mathcal{A} := \sum_{j=1}^{d} \gamma_j \otimes A_j.$$

By assumption, we have that $\mathcal{A} \in \mathcal{I}(\mathbb{C}^{N_d} \otimes \mathcal{H})$. Therefore, since $\gamma_k \otimes 1 \in \mathcal{B}(\mathbb{C}^{N_d} \otimes \mathcal{H})$ and $\mathcal{I}$ is an ideal, it follows that $\mathcal{A}(\gamma_k \otimes 1) + (\gamma_k \otimes 1)\mathcal{A} \in \mathcal{I}(\mathbb{C}^{N_d} \otimes \mathcal{H})$. Moreover, since γ_j anticommutes with γ_k, for all $j \neq k$, have the identity

$$\mathcal{A}(\gamma_k \otimes 1) + (\gamma_k \otimes 1)\mathcal{A} = \sum_{j=1}^{d} (\gamma_j\gamma_k + \gamma_k\gamma_j) \otimes A_j = 2\mathbb{I} \otimes A_k,$$

so $\mathbb{I} \otimes A_k \in \mathcal{I}(\mathbb{C}^{N_d} \otimes \mathcal{H})$.

Let $\mathbf{e}_1 = (1, 0, \ldots, 0) \in \mathbb{C}^{N_d}$, and let $P_{1,1} := \operatorname{diag}(\mathbf{e}_1) \in M_{N_d}(\mathbb{C})$ be the projection of $\mathbb{C}^{N_d}$ onto $\operatorname{span}\{\mathbf{e}_1\}$. Then $P_{1,1} \otimes 1$ is the projection of $\mathbb{C}^{N_d} \otimes \mathcal{H}$ onto $\operatorname{span}\{\mathbf{e}_1\} \otimes \mathcal{H} \simeq \mathcal{H}$ and the restriction of the operator

$$(P_{1,1} \otimes 1)(\mathbb{I} \otimes A_k)(P_{1,1} \otimes 1) = P_{1,1} \otimes A_k$$

to $\operatorname{span}\{\mathbf{e}_1\} \otimes \mathcal{H}$ belongs to $\mathcal{I}\big(\operatorname{span}\{\mathbf{e}_1\} \otimes \mathcal{H}\big)$. Hence, $A_k \in \mathcal{I}(\mathcal{H})$.

(ii). Fix any $k = 1, \ldots, d$. For brevity, let

$$\mathcal{B} := \sum_{j<\ell} \gamma_j\gamma_k \otimes B_{j,\ell}.$$

By assumption, we have that $\mathcal{B} \in \mathcal{I}(\mathbb{C}^{N_d} \otimes \mathcal{H})$. Therefore,

$$\mathcal{B}(\gamma_k \otimes 1) - (\gamma_k \otimes 1)\mathcal{B} \in \mathcal{I}(\mathbb{C}^{N_d} \otimes \mathcal{H}).$$

Moreover, by the anticommutativity of the gamma matrices, we have that

$$\begin{aligned} \mathcal{B}(\gamma_k \otimes 1) - (\gamma_k \otimes 1)\mathcal{B} &= \sum_{j<\ell} (\gamma_j\gamma_\ell\gamma_k - \gamma_k\gamma_j\gamma_\ell) \otimes B_{j,\ell} \\ &= \sum_{j<k} 2\gamma_j \otimes B_{j,k} - \sum_{\ell>k} 2\gamma_k \otimes B_{k,\ell} = \sum_{j=1}^{d} \gamma_\alpha \otimes \widetilde{A}_j, \end{aligned}$$

where

$$\widetilde{A}_j := \begin{cases} 2B_{j,k}, & \text{if } j < k, \\ 0, & \text{if } j = k, \\ -2B_{k,j}, & \text{if } j > k. \end{cases}$$

Hence, applying (i) to $\sum_{j=1}^{d} \gamma_j \otimes \widetilde{A}_j$, we have that $\widetilde{A}_j \in \mathcal{I}(\mathcal{H})$, for every $j = 1, \ldots, d$. In particular, we have that $B_{j,k} \in \mathcal{I}(\mathcal{H})$, for all $j = 1, \ldots, d$ with $j < k$. □

Unlike the case for the algebra of $n \times n$ matrices (for $n \in \mathbb{N}$), the C^*-algebra $\mathcal{B}(\mathcal{H})$ has infinitely many non-trivial two-sided ideals, all of which are subspaces of $\mathcal{K}(\mathcal{H})$ (see, e.g., [75, p. 25], [79, Proposition 2.1]). Motivated by this fact, J. Calkin [15] demonstrated an intrinsic connection between such ideals of operators and certain subspaces of $c_0(\mathbb{N})$. The reader is referred to [79, Chapter 2] for further details.

In the following, for a sequence $c = \{c_n\}_{n\in\mathbb{N}} \in c_0(\mathbb{N})$, we define the *decreasing rearrangement* $\{\mu(j,c)\}_{j\in\mathbb{N}} \in c_0(\mathbb{N})$ of c by the expression

$$\mu(j,c) := \min\Big\{\lambda \in [0,\infty) \,:\, \#\{n \in \mathbb{N} \,:\, |c_n| > \lambda\} \leq j\Big\}.$$

Definition 2.13. A linear subspace $\iota(\mathbb{N})$ of $c_0(\mathbb{N})$ is called a *Calkin space* if for any $c \in c_0(\mathbb{N})$, $d \in \iota(\mathbb{N})$,

$$\mu(j,c) \leq \mu(j,d), \text{ for all } j \in \mathbb{N} \quad \Rightarrow \quad c \in \iota(\mathbb{N}).$$

Suppose $A \in \mathcal{K}(\mathcal{H})$. The *singular value sequence* $\mu(A) = \{\mu(j,A)\}_{j\in\mathbb{N}}$ of A is the unique sequence of non-zero eigenvalues of $|A|$, counting multiplicity, arranged in decreasing order (unless A is finite rank, in which case $\mu(j,A) = 0$ for all $j \geq \operatorname{rank}(A)$).

Theorem 2.14 (Calkin correspondence)**.** [15, Theorem 1.6] *Suppose $\iota(\mathbb{N}) \subset c_0(\mathbb{N})$, and let*

$$\mathcal{I}(\mathcal{H}) := \{A \in \mathcal{K}(\mathcal{H}) \,:\, \mu(A) \in \iota(\mathbb{N})\}.$$

$\mathcal{I}(\mathcal{H})$ is a two-sided ideal of $\mathcal{B}(\mathcal{H})$ if and only if $\iota(\mathbb{N})$ is a Calkin space, and the correspondence $\iota(\mathbb{N}) \leftrightarrow \mathcal{I}(\mathcal{H})$ is a lattice isomorphism (with respect to inclusion) between the Calkin spaces and the two-sided ideals of $\mathcal{B}(\mathcal{H})$.

It is not immediate whether completeness is preserved under the Calkin correspondence. However, it has been shown that a symmetric (quasi-)Banach sequence space corresponds to a (quasi-)Banach ideal of $\mathcal{B}(\mathcal{H})$ (Theorem 2.16 below, see also [57, Chapter 3]).

Definition 2.15. Suppose $\iota(\mathbb{N})$ is a Calkin space. If $\iota(\mathbb{N})$ is (quasi-)Banach with respect to the (quasi-)norm $\|\cdot\|_\iota$ such that

$$\|c\|_\iota \leq \|d\|_\iota, \text{ for all } c \in c_0(\mathbb{N}),\, d \in \iota(\mathbb{N}) \quad \Rightarrow \quad \mu(c) \leq \mu(d),$$

then $(\iota(\mathbb{N}), \|\cdot\|_\iota)$ is called a symmetric (quasi-)Banach sequence space.

Theorem 2.16. *Suppose $\iota(\mathbb{N})$ is a Calkin space equipped with a (quasi-)norm $\|\cdot\|_\iota$, and let $\mathcal{I}(\mathcal{H})$ be its corresponding two-sided ideal of $\mathcal{B}(\mathcal{H})$. Then the function $\|\cdot\|_{\mathcal{I}} : \mathcal{I}(\mathcal{H}) \to [0,\infty)$ defined by the expression*

$$\|A\|_{\mathcal{I}} := \big\|\mu(A)\big\|_\iota, \quad \textit{for } A \in \mathcal{I}(\mathcal{H}). \tag{2.8}$$

is a quasi-norm on $\mathcal{I}(\mathcal{H})$. We have the following:

(*i*) [49] *If* $\big(\iota(\mathbb{N}), \|\cdot\|_\iota\big)$ *is a symmetric Banach sequence space, then* $\|\cdot\|_{\mathcal{I}}$ *is a norm, and* $\big(\mathcal{I}(\mathcal{H}), \|\cdot\|_{\mathcal{I}}\big)$ *is a Banach ideal of* $\mathcal{B}(\mathcal{H})$*.*

(*ii*) [83, Theorem 4] *If* $\big(\iota(\mathbb{N}), \|\cdot\|_\iota\big)$ *is a symmetric quasi-Banach space, then* $\big(\mathcal{I}(\mathcal{H}), \|\cdot\|_{\mathcal{I}}\big)$ *is a quasi-Banach ideal of* $\mathcal{B}(\mathcal{H})$*.*

Example 2.17. The space $c_0(\mathbb{N})$ of sequences converging to zero is a Calkin space whose corresponding two-sided ideal of $\mathcal{B}(\mathcal{H})$ is $\mathcal{K}(\mathcal{H})$. Additionally, the space $c_{00}(\mathbb{N})$ of sequences that are eventually zero is also a Calkin space whose corresponding two-sided ideal of $\mathcal{B}(\mathcal{H})$ is $\mathcal{C}_{00}(\mathcal{H})$.

For $1 \le p < \infty$, the sequence spaces $\ell_p(\mathbb{N})$ and $\ell_{p,\infty}(\mathbb{N})$ are also Calkin spaces. Since

$$c_{00}(\mathbb{N}) \subset \ell_1(\mathbb{N}) \subset \ell_{1,\infty}(\mathbb{N}) \subset \ell_p(\mathbb{N}) \subset \ell_{p,\infty}(\mathbb{N}) \subset \ell_q(\mathbb{N}) \subset \ell_{q,\infty}(\mathbb{N}) \subset c_0(\mathbb{N}),$$

for $1 \le p \le q < \infty$, there exist corresponding two-sided ideals of $\mathcal{B}(\mathcal{H})$, denoted $\mathcal{L}_p(\mathcal{H})$ and $\mathcal{L}_{p,\infty}(\mathcal{H})$ respectively, satisfying

$$\mathcal{C}_{00}(\mathcal{H}) \subset \mathcal{L}_1 \subset \mathcal{L}_{1,\infty} \subset \mathcal{L}_p \subset \mathcal{L}_{p,\infty} \subset \mathcal{L}_q \subset \mathcal{L}_{q,\infty} \subset \mathcal{K}(\mathcal{H}).$$

We shall explore these ideals in further detail in the following few sections.

2.3.1 Schatten ideals

The Schatten ideals are a central example of Banach ideals of $\mathcal{B}(\mathcal{H})$ whose important properties as used in this thesis are gathered below. It is well-known that $\big(\ell_p(\mathbb{N}), \|\cdot\|_p\big)$, for $1 \le p < \infty$, is a symmetric Banach sequence space. Therefore, Theorem 2.16 (*i*) allows us to introduce the corresponding Banach ideals $\mathcal{L}_p(\mathcal{H})$.

Definition 2.18. Suppose $0 < p < \infty$. The *pth Schatten ideal* of $\mathcal{B}(\mathcal{H})$, denoted by $\mathcal{L}_p(\mathcal{H})$ (and sometimes abbreviated as simply $\mathcal{L}_p$), is defined by

$$\mathcal{L}_p(\mathcal{H}) := \big\{A \in \mathcal{K}(\mathcal{H}) \,:\, \mu(A) \in \ell_p(\mathbb{N})\big\}.$$

For $p \ge 1$, $\mathcal{L}_p$ is equipped with the norm defined by

$$\|A\|_p := \big\|\mu(A)\big\|_p, \quad A \in \mathcal{L}_p(\mathcal{H}). \tag{2.9}$$

In particular, $\big(\mathcal{L}_p(\mathcal{H}), \|\cdot\|_p\big)$, for $1 \le p < \infty$, is a Banach ideal of $\mathcal{B}(\mathcal{H})$. Furthermore, since the sequence space $c_{00}(\mathbb{N})$ is dense in $\ell_p(\mathbb{N})$, we have that $\mathcal{C}_{00}(\mathcal{H})$ is dense in $\mathcal{L}_p(\mathcal{H})$ [79, Theorem 2.7].

We also have the following estimates:

Theorem 2.19 (Hölder inequality)**.** [79, Theorem 2.8] *Suppose* $1 \leq p, q, r < \infty$ *such that* $\frac{1}{p} + \frac{1}{q} = \frac{1}{r}$*. If* $A \in \mathcal{L}_p(\mathcal{H})$ *and* $B \in \mathcal{L}_q(\mathcal{H})$*, then* $AB \in \mathcal{L}_r(\mathcal{H})$ *and*

$$\|AB\|_r \leq \|A\|_p \|B\|_q. \tag{2.10}$$

We now state a special case of the three line theorem (see, e.g., [40, p. 136], [79, Theorem 2.9], [82, Corollary 13]), which will be used in Section 3.2 below.

Theorem 2.20. *Suppose* $0 < \alpha < 1$ *and* $1 \leq p < \infty$*. If* $A, B \in \mathcal{B}(\mathcal{H})$ *are self-adjoint such that* $B \geq 0$ *and* $AB \in \mathcal{L}_p(\mathcal{H})$*, then* $B^\alpha A B^{1-\alpha} \in \mathcal{L}_p(\mathcal{H})$ *and*

$$\|B^\alpha A B^{1-\alpha}\|_p \leq \|AB\|_p. \tag{2.11}$$

2.3.2 Weak Schatten ideals and the Dixmier–Macaev ideal

In the following, we consider the Sargent space [64],

$$m_{1,\infty}(\mathbb{N}) \coloneqq \Big\{ (a_j)_{j\in\mathbb{N}} \in \ell_\infty(\mathbb{N}) \,:\, \sum_{j=1}^{n} |a_j| = \mathcal{O}\big(\log(2+n)\big) \Big\}.$$

Note that $m_{1,\infty}(\mathbb{N})$ is a Calkin space such that

$$\ell_{1,\infty}(\mathbb{N}) \subset m_{1,\infty}(\mathbb{N}) \subset \ell_p(\mathbb{N}), \quad \text{for all } p > 1.$$

Moreover, we have that $\big(\ell_{p,\infty}(\mathbb{N}), \|\cdot\|_{p,\infty}\big)$ is a symmetric quasi-Banach sequence space, and $\big(m_{1,\infty}(\mathbb{N}), \|\cdot\|_{m_{1,\infty}}\big)$ is a symmetric Banach sequence space, where

$$\|c\|_{m_{1,\infty}} \coloneqq \sup_{n\in\mathbb{N}} \Big(\frac{\sum_{j=0}^{n} c_j}{\log(2+n)} \Big), \quad \text{for } c = (c_j)_{j\in\mathbb{N}} \in m_{1,\infty}(\mathbb{N}).$$

We may construct the following two-sided ideals of $\mathcal{B}(\mathcal{H})$ via the Calkin correspondence.

Definition 2.21. Let $1 \leq p < \infty$.

- The *pth weak Schatten class* of $\mathcal{B}(\mathcal{H})$ is defined by

$$\mathcal{L}_{p,\infty}(\mathcal{H}) \coloneqq \big\{ A \in \mathcal{K}(\mathcal{H}) \,:\, \mu(A) \in \ell_{p,\infty}(\mathbb{N}) \big\}.$$

- The *Dixmier–Macaev class* of $\mathcal{B}(\mathcal{H})$ (also referred to as the *dual of the Macaev ideal*) is defined by

$$\mathcal{M}_{1,\infty}(\mathcal{H}) \coloneqq \big\{ A \in \mathcal{K}(\mathcal{H}) \,:\, \mu(A) \in m_{1,\infty}(\mathbb{N}) \big\}.$$

By Theorem 2.16, the space $\mathcal{L}_{p,\infty}(\mathcal{H})$, for $1 \leq p < \infty$, forms a quasi-Banach ideal of $\mathcal{K}(\mathcal{H})$ when equipped with the associated quasi-norm

$$\|A\|_{p,\infty} \coloneqq \big\|\mu(A)\big\|_{p,\infty}, \quad A \in \mathcal{L}_{p,\infty}(\mathcal{H}),$$

while $\mathcal{M}_{1,\infty}(\mathcal{H})$ forms a Banach ideal when equipped with the associated norm

$$\|A\|_{\mathcal{M}_{1,\infty}} := \big\|\mu(A)\big\|_{m_{1,\infty}}, \quad A \in \mathcal{M}_{1,\infty}(\mathcal{H}).$$

By Theorem 2.14, these ideals admit the following nesting:

$$\mathcal{L}_{1,\infty}(\mathcal{H}) \subset \mathcal{M}_{1,\infty}(\mathcal{H}) \subset \mathcal{L}_p(\mathcal{H}), \quad \text{for all } p > 1.$$

Definition 2.22. Suppose $\mathcal{I}$ is a quasi-Banach ideal of $\mathcal{B}(\mathcal{H})$. The *separable part* of $\mathcal{I}$, denoted $\mathcal{I}_0$, is the $\|\cdot\|_{\mathcal{I}}$-closure of $\mathcal{C}_{00}(\mathcal{H})$ in $\mathcal{I}$.

The weak Schatten classes (as well as their separable parts) admit their own versions of the Hölder inequality.

Theorem 2.23. [79, Theorem 2.8] *Let* $1 \le p, q, r < \infty$ *such that* $\frac{1}{p} + \frac{1}{q} = \frac{1}{r}$.

(*i*) *If* $A \in \mathcal{L}_{p,\infty}(\mathcal{H})$ *and* $B \in \mathcal{L}_{q,\infty}(\mathcal{H})$, *then* $AB \in \mathcal{L}_{r,\infty}(\mathcal{H})$.

(*ii*) *If* $A \in \big(\mathcal{L}_{p,\infty}(\mathcal{H})\big)_0$ *and* $B \in \mathcal{L}_{q,\infty}(\mathcal{H})$, *then* $AB \in \big(\mathcal{L}_{r,\infty}(\mathcal{H})\big)_0$.

2.4 Traces on ideals

In this section we introduce the notion of traces on ideals of $\mathcal{B}(\mathcal{H})$, and recall the definitions of the classical trace on $\mathcal{L}_1$ and the Dixmier traces on $\mathcal{L}_{1,\infty}$ and $\mathcal{M}_{1,\infty}$.

Definition 2.24. Let $\mathcal{H}$ be a separable Hilbert space, and suppose $\mathcal{I}$ is a two-sided ideal of $\mathcal{B}(\mathcal{H})$. A linear functional $\varphi : \mathcal{I} \to \mathbb{C}$ is called a *trace* if φ is unitarily invariant; that is,

$$\varphi(U^{-1}AU) = \varphi(A), \quad \text{for all } A \in \mathcal{I}, \text{ and any unitary } U \in \mathcal{B}(\mathcal{H}).$$

Note that these traces may be equivalently characterised using the cyclic property:

Proposition 2.25 (Tracial cyclicity)**.** [57, Lemma 1.2.11] *A linear functional* φ *on the two-sided ideal* $\mathcal{I}$ *is a trace if and only if*

$$\varphi\big([A, B]\big) = 0, \quad \textit{for all } A \in \mathcal{I},\ B \in \mathcal{B}(\mathcal{H}).$$

This result generalises the cyclic property of traces; that is, for complex-valued $n \times n$ matrices $A, B \in M_n(\mathbb{C})$, for $n \in \mathbb{N}$, we have $\operatorname{tr}(AB) = \operatorname{tr}(BA)$.

Definition 2.26. Suppose $\mathcal{I}$ is a quasi-Banach ideal of $\mathcal{B}(\mathcal{H})$, and suppose φ is a trace on $\mathcal{I}$.

- If $\varphi \in \mathcal{I}^*$, then φ is called a *continuous trace.*

- If $\varphi(\sup_\alpha A_\alpha) = \sup_\alpha \varphi(A_\alpha)$ for every bounded increasing directed family of positive operators $\{A_\alpha\}_\alpha$, then φ is called a *normal trace*.

- If φ vanishes on $\mathcal{C}_{00}(\mathcal{H})$, then φ is called a *singular trace*.

Remark 2.27. [57, Lemma 2.6.12] Suppose $\mathcal{I}$ is a quasi-Banach ideal of $\mathcal{B}(\mathcal{H})$, and suppose φ is a continuous trace on $\mathcal{I}$. Then φ is a singular trace if and only if φ vanishes on $\mathcal{I}_0$.

2.4.1 The classical trace

The following form of the classical operator trace is derived from the work of J. von Neumann [58].

Definition 2.28. Suppose $A \in \mathcal{L}_1(\mathcal{H})$. The *classical trace* of A, denoted $\mathrm{Tr}(A)$, is given by the expression

$$\mathrm{Tr}(A) := \sum_{k\in\mathbb{N}} \langle Ae_k, e_k\rangle_{\mathcal{H}},$$

where $\{e_k\}_{k\in\mathbb{N}}$ is some orthonormal basis for $\mathcal{H}$.

Heuristically, the classical trace generalises the procedure of taking the sum of diagonal entries of a finite-dimensional matrix.

Remark 2.29. It follows from the Schur decomposition [79, Theorem 1.4] that Tr is well-defined on $\mathcal{L}_1(\mathcal{H})$, and does not depend upon the choice of orthonormal basis for $\mathcal{H}$ (that is, Tr is unitary invariant). We describe $A \in \mathcal{L}_1$ as being *trace-class*.

Analogous to the finite-dimensional trace, the classical trace of a trace-class operator is given by the sum of its eigenvalues.

Theorem 2.30 (Lidskiĭ theorem)**.** [54] *If $A \in \mathcal{L}_1(\mathcal{H})$, then*

$$\mathrm{Tr}(A) = \sum_j \lambda(j, A),$$

where $\big\{\lambda(j, A)\big\}_j$ is a sequence listing all non-zero eigenvalues of A, counting multiplicity, arranged in an order of decreasing magnitude.

Remark 2.31. Suppose $1 \le p < \infty$. The $\mathcal{L}_p$-norm may be expressed in terms of the classical trace by

$$\|A\|_p = \mathrm{Tr}\left(|A|^p\right)^{\frac{1}{p}}, \quad A \in \mathcal{L}_p(\mathcal{H}). \tag{2.12}$$

It is obvious that the classical trace is not a singular trace. In fact, there are no non-trivial continuous singular traces on $\mathcal{L}_1$, since $(\mathcal{L}_1)_0 = \mathcal{L}_1$. There are, however, many such singular traces on $\mathcal{L}_{1,\infty}$. We describe a certain class of singular non-normal traces on $\mathcal{L}_{1,\infty}$, the Dixmier traces, in the next section.

We shall need the following formula for the trace of a trace-class integral operator in Section 3.4.3 below.

Proposition 2.32. [33, Theorem V.3.1.1], [14, Theorem 3.1] *Suppose the trace-class operator $A \in \mathcal{L}_1\big(L_2(\mathbb{R}^d)\big)$ has integral kernel $K \in L_2(\mathbb{R}^d \times \mathbb{R}^d)$. If K is continuous on $\mathbb{R}^d \times \mathbb{R}^d$, then*

$$\int_{\mathbb{R}^d} K(\mathbf{x},\mathbf{x})\,\mathrm{d}\mathbf{x} < \infty$$

and

$$\mathrm{Tr}(A) = \int_{\mathbb{R}^d} K(\mathbf{x},\mathbf{x})\,\mathrm{d}\mathbf{x}.$$

2.4.2 Dixmier traces

In this section, we shall follow the approach of J. Dixmier [31], who constructed an important example of a normalised singular trace on $\mathcal{M}_{1,\infty}$ that is non-normal (where this latter notion of 'normal' is meant in the sense of Definition 2.26 above). Recall that, by definition, the partial sums for the singular value sequence of an operator $A \in \mathcal{M}_{1,\infty}(\mathcal{H})$ satisfy the property

$$\Big(\frac{1}{\log(2+j)}\sum_{k=0}^{j}\mu(k,A)\Big)_{j\in\mathbb{N}} \in \ell_\infty(\mathbb{N}).$$

Though this sequence may not converge, we may assign a number to this sequence using the notion of an extended limit.

Definition 2.33. A linear functional $\omega \in \ell_\infty(\mathbb{N})^*$ is an *extended limit* if;

(*i*) ω is positive;

(*ii*) $\omega(\mathbf{1}) = 1$, where $\mathbf{1} = (1,1,1,\ldots) \in \ell_\infty(\mathbb{N})$, and;

(*iii*) $\omega(x) = 0$, for every $x \in c_0(\mathbb{N})$.

Remark 2.34. Extended limits are Hahn–Banach extensions of the notion of a limit (in fact, the Hahn–Banach theorem implies there are uncountably many of such extended limits).

Note that the expression

$$\omega\bigg(\Big(\frac{1}{\log(2+j)}\sum_{k=0}^{j}\mu(k,A)\Big)_{j\in\mathbb{N}}\bigg), \quad A \in \mathcal{M}_{1,\infty}$$

is not guaranteed to define an additive linear functional on $\mathcal{M}_{1,\infty}$. This may be resolved if we place the following additional restriction on our choice of ω:

Definition 2.35. For $k \geq 1$, let $\sigma_k : \ell_\infty(\mathbb{N}) \to \ell_\infty(\mathbb{N})$ be the mapping defined by

$$\sigma_k(x_0, x_1, \dots) := (\underbrace{x_0, \dots, x_0}_{k \text{ times}}, \underbrace{x_1, \dots, x_1}_{k \text{ times}}, \dots).$$

The semigroup generated by these maps is called the *dilation semigroup*. We therefore call an extended limit $\omega \in \ell_\infty(\mathbb{N})^*$ a *dilation-invariant extended limit* if it is invariant with respect to the dilation semigroup; that is, if

$$\omega(x) = (\omega \circ \sigma_k)(x), \quad \text{for all } x \in \ell_\infty(\mathbb{N}) \text{ and all } k \geq 1.$$

The existence of dilation-invariant extended limits is known [57, Corollary 6.2.6].

Definition 2.36. Let ω be an extended limit. Let $\mathrm{Tr}_\omega : (\mathcal{M}_{1,\infty})_+ \to \mathbb{C}$ be defined by setting

$$\mathrm{Tr}_\omega(A) = \omega\Big(\Big(\frac{1}{\log(2+j)} \sum_{k=0}^{j} \mu(k, A)\Big)_{j \in \mathbb{N}}\Big), \quad 0 \leq A \in \mathcal{M}_{1,\infty}.$$

Theorem 2.37. *Suppose ω is an extended limit on $\ell_\infty(\mathbb{N})$. We have the following:*

(*i*) [57, Theorem 1.3.1] *The restriction of* Tr_ω *to the positive cone $(\mathcal{L}_{1,\infty})_+$ is both positive and additive, and extends to a linear trace on $\mathcal{L}_{1,\infty}$.*

(*ii*) [24, §IV.2.β], [32, Example 2.5], [57, Theorem 6.3.6] *If ω is dilation-invariant, then* Tr_ω *is positive and additive on $(\mathcal{M}_{1,\infty})_+$, and extends to a linear trace on $\mathcal{M}_{1,\infty}$.*

Given an extended limit ω, the functional Tr_ω on $\mathcal{L}_{1,\infty}$ is called a *Dixmier trace* on $\mathcal{L}_{1,\infty}$. Likewise, given a dilation-invariant extended limit, the functional Tr_ω on $\mathcal{M}_{1,\infty}$ is called a *Dixmier trace* on $\mathcal{M}_{1,\infty}$.

Remark 2.38. Suppose ω is an extended limit on $\ell_\infty(\mathbb{N})$. Observe that, for $A \in \mathcal{L}_1$, we have that

$$0 \leq \lim_{j\to\infty} \frac{1}{\log(2+j)} \sum_{k=0}^{j} \mu(k, A) \overset{(2.9)}{\leq} \lim_{j\to\infty} \frac{\|A\|_1}{\log(2+j)} = 0.$$

Hence, Tr_ω is a singular trace on $\mathcal{L}_{1,\infty}$, since it vanishes on $\mathcal{L}_1$ and, by density, on $(\mathcal{L}_{1,\infty})_0$. Likewise, if ω is dilation-invariant, then Tr_ω is a singular trace on $\mathcal{M}_{1,\infty}$.

In fact, every Dixmier trace on $\mathcal{L}_{1,\infty}$ is just the restriction of a Dixmier trace on $\mathcal{M}_{1,\infty}$, as the following theorem shows.

Theorem 2.39. [57, Lemma 9.7.4] *For every extended limit ω, there exists a dilation-invariant extended limit ω_0 such that*

$$\mathrm{Tr}_\omega(A) = \mathrm{Tr}_{\omega_0}(A), \quad \textit{for all } A \in \mathcal{L}_{1,\infty}.$$

Definition 2.40. An operator $A \in \mathcal{M}_{1,\infty}$ (resp. $A \in \mathcal{L}_{1,\infty}$) is said to be *Dixmier measurable* if $\mathrm{Tr}_{\omega_1}(A) = \mathrm{Tr}_{\omega_2}(A)$, for all dilation-invariant extended limits (resp. extended limits) ω_1, ω_2.

2.5 Examples of operators in (weak) Schatten classes

2.5.1 The Dirichlet Laplacian and its eigenvalues

Definition 2.41. Suppose $\Omega \subset \mathbb{R}^d$ is an open set. Consider the densely-defined positive operator $-\Delta|_{C^\infty_{\mathrm{com}}(\Omega)} : C^\infty_{\mathrm{com}}(\Omega) \to C^\infty_{\mathrm{com}}(\Omega)$ on the Hilbert space $L_2(\Omega)$ defined by the expression

$$\big(-\Delta|_{C^\infty_{\mathrm{com}}(\Omega)}\big) f := -\sum_{k=1}^{d} \frac{\partial^2 f}{\partial x_k^2}, \quad f \in C^\infty_{\mathrm{com}}(\Omega).$$

The self-adjoint extension of $-\Delta|_{C^\infty_{\mathrm{com}}(\Omega)}$ obtained via the Friedrichs extension (see, e.g., [70, Theorem X.23]) is called the *Dirichlet Laplacian for* Ω, and is denoted by $-\Delta^\Omega_{\mathrm{D}}$.

Let $n \in \mathbb{N}$, and suppose $\Omega \subset \mathbb{R}^d$ is an open connected bounded set. We shall say that Ω has *smooth boundary* if there exists a C^∞ function $f : \mathbb{S}^{d-1} \to \mathbb{R}^d$ such that $f(\mathbb{S}^{d-1}) = \partial\Omega$, where $\mathbb{S}^{d-1}$ denotes the unit hypersphere in $\mathbb{R}^d$. Note that every open connected bounded set with smooth boundary is Jordan-contented (in the sense of [71, p. 271], see also [26, pp. 370, 518]).

Remark 2.42. [71, p. 255] Suppose $\Omega \subset \mathbb{R}^d$ is an open connected bounded set with smooth boundary. Then $-\Delta^\Omega_{\mathrm{D}}$ has discrete spectrum, and

$$(1 - \Delta^\Omega_{\mathrm{D}})^{-1} \in \mathcal{K}\big(L_2(\Omega)\big).$$

For open connected bounded subsets $\Omega \subset \mathbb{R}^d$ with smooth boundary, we define the function $\mathcal{N}_\Omega : [0, \infty) \to \mathbb{N} \cup \{\infty\}$ via the Borel functional calculus by

$$\mathcal{N}_\Omega(\lambda) := \mathrm{rank}\,\big(\chi_{[0,\lambda)}(-\Delta^\Omega_{\mathrm{D}})\big), \quad \lambda \geq 0,$$

where $\chi_{[0,\lambda)}$ is the characteristic function of the interval $[0, \lambda)$ (see Definition 2.47 below). $\mathcal{N}_\Omega$ counts how many eigenvalues of $-\Delta^\Omega_{\mathrm{D}}$, with multiplicity, are less than λ. The asymptotic behaviour of $\mathcal{N}_\Omega$ is described by the celebrated Weyl law, of which we write the following special case for Dirichlet Laplacians over open connected bounded sets with smooth boundary.

Theorem 2.43 (Weyl law)**.** [71, Theorem XIII.78] *Suppose $\Omega \subset \mathbb{R}^d$ is an open connected bounded set with smooth boundary. Then*

$$\lim_{\lambda \to \infty} \frac{\mathcal{N}_\Omega(\lambda)}{\lambda^{\frac{d}{2}}} = \frac{\mathrm{Vol}(\mathbb{S}^{d-1})\mathsf{m}(\Omega)}{(2\pi)^d}, \tag{2.13}$$

where $\mathrm{Vol}(\mathbb{S}^{d-1})$ *denotes the geometric volume of* $\mathbb{S}^{d-1}$.

Proposition 2.44. *Suppose* $\Omega \subset \mathbb{R}^d$ *is an open connected bounded set with smooth boundary. Then, for every* $p \geq 1$, *we have that* $(1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2p}} \in \mathcal{L}_{p,\infty}\big(L_2(\Omega)\big)$. *Furthermore,*

$$\mathrm{Tr}_\omega\left((1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2}}\right) = \frac{\mathrm{Vol}(\mathbb{S}^{d-1})\mathsf{m}(\Omega)}{(2\pi)^d},$$

where ω *is any extended limit on* $\ell_\infty(\mathbb{N})$.

Proof. Rearranging Theorem 2.43 above and taking the power of $\frac{1}{p}$ yields

$$\lim_{\lambda\to\infty} \mathcal{N}_\Omega(\lambda)^{\frac{1}{p}}(1+\lambda)^{-\frac{d}{2p}} = C_{d,\Omega}^{\frac{1}{p}}, \tag{2.14}$$

where $C_{d,\Omega} := (2\pi)^{-d}\,\mathrm{Vol}(\mathbb{S}^{d-1})\mathsf{m}(\Omega)$.

Since $(1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2p}}$ is positive, the singular values of $(1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2p}}$ coincide with its eigenvalues. Moreover, since $-\Delta_{\mathrm{D}}^{\Omega}$ has discrete spectrum, the Borel functional calculus [69, Theorem VIII.5] implies that all eigenvalues of $-\Delta_{\mathrm{D}}^{\Omega}$, counting multiplicity, may be ordered by

$$\lambda_j := -1 + \mu\big(j, (1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2p}}\big)^{-\frac{2p}{d}} \in \sigma(-\Delta_{\mathrm{D}}^{\Omega}) \subset [0,\infty), \quad j \in \mathbb{N}.$$

Since $\mu\big((1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2p}}\big)$ is nonnegative, decreasing and converging to zero by construction, we have that $\{\lambda_j\}_{j\in\mathbb{N}}$ is nonnegative, increasing and unbounded. Hence,

$$\mathcal{N}_\Omega(\lambda_j) \sim 1+j, \quad \text{as } j \to \infty.$$

Substituting $\lambda = \lambda_j$ in (2.14) above then yields

$$\lim_{j\to\infty}(1+j)^{\frac{1}{p}}\mu\big(j,(1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2p}}\big) = C_{d,\Omega}^{\frac{1}{p}}.$$

Hence, by the definition of $\ell_{p,\infty}(\mathbb{N})$, we have that $(1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2p}} \in \mathcal{L}_{p,\infty}\big(L_2(\Omega)\big)$.

Next, setting $p=1$, observe that for all $\varepsilon > 0$, there exists $N_\varepsilon > 0$ such that

$$\left|\mu\big(j,(1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2}}\big) - \frac{C_{d,\Omega}}{1+j}\right| < \frac{\varepsilon}{1+j}, \quad \text{for all } j \geq N_\varepsilon.$$

Summing up over $j = N_\varepsilon,\dots,N$, for any $N \geq N_\varepsilon$, dividing through by $\log(2+N)$ and taking the limit as $N\to\infty$, we observe that

$$\left|\lim_{N\to\infty}\frac{\sum_{j=N_\varepsilon}^{N}\mu\big(j,(1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2}}\big)}{\log(2+N)} - C_{d,\Omega}\right| < \varepsilon.$$

Therefore

$$\begin{aligned}\left|\mathrm{Tr}_\omega\left((1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2}}\right) - C_{d,\Omega}\right| \leq{}& \left|\lim_{N\to\infty}\frac{\sum_{j=0}^{N_\varepsilon}\mu\big(j,(1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2}}\big)}{\log(2+N)}\right| \\ &+ \left|\lim_{N\to\infty}\frac{\sum_{j=N_\varepsilon}^{N}\mu\big(j,(1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2}}\big)}{\log(2+N)} - C_{d,\Omega}\right| < \varepsilon.\end{aligned}$$

Finally, since ε is arbitrary, we conclude that

$$\mathrm{Tr}_\omega\big((1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2}}\big) = C_{d,\Omega}. \qquad \square$$

2.5.2 Cwikel estimates

In the previous section, we saw that for open connected bounded sets $\Omega \subset \mathbb{R}^d$ with smooth boundary, the Bessel potential $(1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{p}}$ belongs to the weak Schatten class $\mathcal{L}_{p,\infty}\big(L_2(\Omega)\big)$, where $-\Delta_{\mathrm{D}}^{\Omega}$ denotes the Dirichlet Laplacian for Ω. However, for unbounded Ω, the operator $(1-\Delta_{\mathrm{D}}^{\Omega})^{-\frac{d}{2p}}$ is not necessarily compact. For example, the Laplacian Δ over $\mathbb{R}^d$ has purely absolutely continuous spectrum $\sigma(-\Delta) = [0,\infty)$, so $(1-\Delta)^{-\frac{d}{2p}}$ cannot be compact.

However, there exist sufficient conditions on functions $f, g \in L_{2,\mathrm{loc}}(\mathbb{R}^d)$ such that the operator

$$M_f g(\nabla) := M_f \mathcal{F}^{-1} M_g \mathcal{F}$$

defined on the domain

$$\mathrm{dom}\big(M_f g(\nabla)\big) := \Big\{ h \in \mathcal{S}(\mathbb{R}^d) \,:\, \big\| f \cdot \mathcal{F}^{-1}(g \cdot \hat{h})\big\|_2 + \|g \cdot \hat{h}\|_2 < \infty \Big\}$$

extends to a compact operator on $L_2(\mathbb{R}^d)$ belonging to a (weak) Schatten ideal.

Theorem 2.45. [77, Theorem 2.1], [72, Theorem XI.20], [79, Theorem 4.1] *Suppose* $2 \leq p < \infty$. *If* $f, g \in L_p(\mathbb{R}^d)$, *then* $M_f g(\nabla) \in \mathcal{L}_p$ *and*

$$\big\| M_f g(\nabla) \big\|_p \leq \mathrm{const}_p \cdot \|f\|_p \|g\|_p.$$

The following estimate for weak Schatten classes was first conjectured by B. Simon in [78, Conjecture 1] and proved by M. Cwikel in 1977.

Theorem 2.46. [27], [72, Theorem XI.22], [79, Theorem 4.2] *Suppose* $2 < p < \infty$. *If* $f \in L_p(\mathbb{R}^d)$ *and* $g \in L_{p,\infty}(\mathbb{R}^d)$, *then* $M_f g(\nabla) \in \mathcal{L}_{p,\infty}$ *and*

$$\big\| M_f g(\nabla) \big\|_{p,\infty} \leq \mathrm{const}_p \cdot \|f\|_p \|g\|_{p,\infty}.$$

For $1 \leq p < 2$, the estimates are quite different. We define the following function spaces in the style of M. Birman and M. Solomyak [10, 12]:

Definition 2.47. Let $\mathscr{Q}_{\mathbf{n}}$ denote the unit cube centered at $\mathbf{n} \in \mathbb{Z}^d$. For a region $\Omega \subset \mathbb{R}^d$, denote by $\chi_\Omega : \mathbb{R}^d \to \{0,1\}$ the *characteristic function* of Ω; that is, for $\mathbf{x} \in \mathbb{R}^d$,

$$\chi_\Omega(\mathbf{x}) = \begin{cases} 1, & \text{if } \mathbf{x} \in \Omega, \\ 0, & \text{otherwise.} \end{cases}$$

Then, for $1 \le p < 2$, $1 \le q \le \infty$, let

$$\ell_p(L_q)(\mathbb{R}^d) := \left\{ f \in L_0(\mathbb{R}^d) \ : \ \sum_{\mathbf{n}\in\mathbb{Z}^d} \|f\chi_{\mathscr{Q}_\mathbf{n}}\|_q^p < \infty \right\}$$

denote *Birman–Solomyak space* with the corresponding norm

$$\|f\|_{\ell_p(L_q)} := \left(\sum_{\mathbf{n}\in\mathbb{Z}^d} \|f\chi_{\mathscr{Q}_\mathbf{n}}\|_q^p \right)^{\frac{1}{p}}, \qquad f \in \ell_p(L_q)(\mathbb{R}^d). \tag{2.15}$$

Remark 2.48. If $f \in \ell_p(L_q)(\mathbb{R}^d)$ and $0 < r < 1$, then $|f|^r \in \ell_{\frac{p}{r}}(L_{\frac{q}{r}})(\mathbb{R}^d)$, since

$$\big\| \, |f|^r \big\|_{\ell_{\frac{p}{r}}(L_{\frac{q}{r}})}^{\frac{1}{r}} = \|f\|_{\ell_p(L_q)}. \tag{2.16}$$

Remark 2.49. If $1 \le p \le 2$, then for all $\alpha > \frac{d}{p}$,

$$\langle \cdot \rangle^{-\alpha} \in \ell_p(L_2)(\mathbb{R}^d).$$

Theorem 2.50. [10], [79, Theorem 4.5] *Suppose* $1 \le p \le 2$. *If* $f, g \in \ell_p(L_2)(\mathbb{R}^d)$, *then* $M_f g(\nabla) \in \mathcal{L}_p$ *and*

$$\big\| M_f g(\nabla) \big\|_p \le \mathrm{const}_p \cdot \|f\|_{\ell_p(L_2)} \|g\|_{\ell_p(L_2)}.$$

Next, for $1 \le p \le 2$ and $1 \le q \le \infty$, define a weak variant of Birman–Solomyak space as in [79, p. 9] by

$$\ell_{p,\infty}(L_q)(\mathbb{R}^d) := \left\{ f \in L_0(\mathbb{R}^d) \ : \ \Big\| \big\{ \|f\chi_{\mathscr{Q}_\mathbf{n}}\|_q \big\}_{\mathbf{n}\in\mathbb{Z}^d} \Big\|_{p,\infty} < \infty \right\}.$$

with associated quasi-norm

$$\|f\|_{\ell_{p,\infty}(L_q)} := \Big\| \big\{ \|f\chi_{\mathscr{Q}_\mathbf{n}}\|_q \big\}_{\mathbf{n}\in\mathbb{Z}^d} \Big\|_{p,\infty}.$$

Remark 2.51. If $1 \le p \le 2$, then for all $\alpha \ge \frac{d}{p}$,

$$\langle \cdot \rangle^{-\alpha} \in \ell_{p,\infty}(L_2)(\mathbb{R}^d).$$

Theorem 2.52. [7, 5.7 (p. 103)] *Suppose* $1 \le p < 2$. *If* $f \in \ell_p(L_2)(\mathbb{R}^d)$ *and* $g \in \ell_{p,\infty}(L_2)(\mathbb{R}^d)$, *then* $M_f g(\nabla) \in \mathcal{L}_{p,\infty}$ *and*

$$\big\| M_f g(\nabla) \big\|_{p,\infty} \le \mathrm{const}_p \cdot \|f\|_{\ell_p(L_2)} \|g\|_{\ell_{p,\infty}(L_2)}$$

Unlike the case for the Schatten classes, the case $\mathcal{L}_{2,\infty}$ is a boundary case, and special care must be taken to construct Cwikel estimates therein (see, e.g., [53, Theorem 5.6]).

In order to simplify the assumptions in Chapter 4, we seek Sobolev spaces strictly contained in Birman–Solomyak spaces (see Proposition 2.55 below). For brevity, if $f \in C^0(\mathbb{R}^d)$ and $k = 1, \ldots, d$, we adopt the convention

$$f(\mathbf{t}_k; \mathbf{x}_{d-k}) := f(t_1, \ldots, t_k, x_{k+1}, \ldots, x_d),$$

$$\text{where } \mathbf{t}_k = (t_1, \ldots, t_k) \in \mathbb{R}^k, \ \mathbf{x}_{d-k} = (x_{k+1}, \ldots, x_d) \in \mathbb{R}^{d-k}.$$

Lemma 2.53. *Let $\mathscr{Q}_{\mathbf{0}} = [-\frac{1}{2}, \frac{1}{2}]^d \subset \mathbb{R}^d$, and suppose $f \in C^d(\mathscr{Q}_{\mathbf{0}})$. For every $k = 1, \ldots, d$,*

$$\big|f(\mathbf{x})\big| \leq \sum_{\boldsymbol{\alpha}\in\{0,1\}^k} \int_{[-\frac{1}{2},\frac{1}{2}]^k} \big|\nabla^{\boldsymbol{\alpha}} f(\mathbf{t}_k; \mathbf{x}_{d-k})\big| \,\mathrm{d}\mathbf{t}_k, \tag{2.17}$$

for all $\mathbf{x} = (x_1, \ldots, x_d) \in \mathscr{Q}_{\mathbf{0}}$, and where $\mathbf{x}_{d-k} = (x_{k+1}, \ldots, x_d)$.

Proof. Firstly, for $-\infty < a < b < \infty$, recall that if g is a C^1 function on the interval $[a, b] \subset \mathbb{R}$, then the mean value theorem and the fundamental theorem of calculus imply that

$$\big|g(x)\big| \leq \int_a^b \Big|\frac{\mathrm{d}g(t)}{\mathrm{d}t}\Big| \,\mathrm{d}t + \int_a^b \big|g(t)\big| \,\mathrm{d}t, \quad \text{for all } x \in [a, b]. \tag{2.18}$$

We now prove the lemma inductively. The estimate for $k = 1$ follows from (2.18); for every $-\frac{1}{2} \leq x_2, \ldots, x_d \leq \frac{1}{2}$, the expression $f(\,\cdot\,; \mathbf{x}_{d-1})$ defines a C^1 function on the interval $[-\frac{1}{2}, \frac{1}{2}]$, so we observe that

$$\big|f(\mathbf{x})\big| \leq \int_{-\frac{1}{2}}^{\frac{1}{2}} \big|\partial_1 f(t_1; \mathbf{x}_{d-1})\big| \,\mathrm{d}t_1 + \int_{-\frac{1}{2}}^{\frac{1}{2}} \big|f(t_1; \mathbf{x}_{d-1})\big| \,\mathrm{d}t_1.$$

Suppose now that (2.17) holds for some $1 \leq k < d$. For each $\boldsymbol{\alpha} \in \{0, 1\}^k$ and every $-\frac{1}{2} \leq x_1, \ldots, x_k, x_{k+2}, \ldots, x_d \leq \frac{1}{2}$, the expression

$$\nabla^{\boldsymbol{\alpha}} f(\mathbf{x}_k;\,\cdot\,; \mathbf{x}_{d-k-1}) = \nabla^{\boldsymbol{\alpha}} f(x_1, \ldots, x_k, \,\cdot\,, x_{k+2}, \ldots, x_d)$$

defines a C^1 function on $[-\frac{1}{2}, \frac{1}{2}]$. Hence, we may apply (2.18) to obtain the estimate

$$\begin{aligned}
&\sum_{\boldsymbol{\alpha}\in\{0,1\}^k} \int_{[-\frac{1}{2},\frac{1}{2}]^k} \big|\nabla^{\boldsymbol{\alpha}} f(\mathbf{t}_k; x_{k+1}; \mathbf{x}_{d-k-1})\big| \,\mathrm{d}\mathbf{t}_k \\
&\overset{(2.18)}{\leq} \sum_{\boldsymbol{\alpha}\in\{0,1\}^k} \int_{[-\frac{1}{2},\frac{1}{2}]^k} \bigg(\int_{[-\frac{1}{2},\frac{1}{2}]} \big|\nabla^{\boldsymbol{\alpha}} f(\mathbf{t}_k; t_{k+1}; \mathbf{x}_{d-k-1})\big| \mathrm{d}t_{k+1} \\
&\qquad\qquad + \int_{[-\frac{1}{2},\frac{1}{2}]} \big|\nabla^{\boldsymbol{\alpha}} \partial_{k+1} f(\mathbf{t}_k; t_{k+1}; \mathbf{x}_{d-k-1})\big| \,\mathrm{d}t_{k+1} \bigg) \,\mathrm{d}\mathbf{t}_k \\
&= \sum_{\boldsymbol{\alpha}\in\{0,1\}^{k+1}} \int_{[-\frac{1}{2},\frac{1}{2}]^{k+1}} \big|\nabla^{\boldsymbol{\alpha}} f(\mathbf{t}_{k+1}; \mathbf{x}_{d-k})\big| \mathrm{d}\mathbf{t}_{k+1},
\end{aligned}$$

as required. ☐

Lemma 2.54. *Suppose $f \in C_{\mathrm{b}}^d(\mathbb{R}^d)$ and $1 \leq p < 2$. Then, for all $\mathbf{n} \in \mathbb{Z}^d$,*

$$\|f\chi_{\mathscr{Q}_{\mathbf{n}}}\|_\infty \leq \text{const} \cdot \Big(\sum_{\boldsymbol{\alpha}\in\{0,1\}^d} \big\|(\nabla^{\boldsymbol{\alpha}} f)\chi_{\mathscr{Q}_{\mathbf{n}}}\big\|_p^p \Big)^{\frac{1}{p}}. \tag{2.19}$$

Proof. Without loss of generality, we prove the result for $\mathbf{n} = \mathbf{0}$. Observe that, for all $x \in \mathscr{Q}$, appealing to Theorem 2.53 for $k = d$ yields

$$\big|f(x)\big| \leq \sum_{\boldsymbol{\alpha}\in\{0,1\}^d} \int_{[-\frac{1}{2},\frac{1}{2}]^d} \big|\nabla^{\boldsymbol{\alpha}} f(\mathbf{t})\big| \,\mathrm{d}\mathbf{t} = \sum_{\boldsymbol{\alpha}\in\{0,1\}^d} \big\|(\nabla^{\boldsymbol{\alpha}} f)\chi_{\mathscr{Q}}\big\|_1.$$

Therefore, since $x \in \mathscr{Q}$ is arbitrary, if $2 < r \leq \infty$ such that $1 = \frac{1}{p} + \frac{1}{r}$, then the Hölder inequality gives the estimate

$$\|f\chi_{\mathscr{Q}}\|_\infty \leq \sum_{\boldsymbol{\alpha}\in\{0,1\}^d} \big\|(\nabla^{\boldsymbol{\alpha}} f)\chi_{\mathscr{Q}}\big\|_1 \leq \sum_{\boldsymbol{\alpha}\in\{0,1\}^d} \|\chi_{\mathscr{Q}}\|_r \big\|(\nabla^{\boldsymbol{\alpha}} f)\chi_{\mathscr{Q}}\big\|_p.$$

Appealing once more to the Hölder inequality then gives

$$\|f\chi_{\mathscr{Q}}\|_\infty \leq \Big(\sum_{\boldsymbol{\alpha}\in\{0,1\}^d} \|\chi_{\mathscr{Q}}\|_r^r\Big)^{\frac{1}{r}} \Big(\sum_{\boldsymbol{\alpha}\in\{0,1\}^d} \big\|(\nabla^{\boldsymbol{\alpha}} f)\chi_{\mathscr{Q}}\big\|_p^p\Big)^{\frac{1}{p}} = 2^{\frac{d}{r}} \Big(\sum_{\boldsymbol{\alpha}\in\{0,1\}^d} \big\|(\nabla^{\boldsymbol{\alpha}} f)\chi_{\mathscr{Q}}\big\|_p^p\Big)^{\frac{1}{p}}. \square$$

Proposition 2.55. *If $1 \leq p < 2$ and $1 \leq q < \infty$, then $W_p^d(\mathbb{R}^d) \subset \ell_p(L_q)(\mathbb{R}^d)$ and*

$$\|f\|_{\ell_p(L_q)} \leq \mathrm{const} \cdot \|f\|_{W_p^d}, \quad \text{for all } f \in W_p^d(\mathbb{R}^d).$$

Proof. Let $f \in W_p^d(\mathbb{R}^d) \cap C_{\mathrm{b}}^d(\mathbb{R}^d)$. By Lemma 2.54 and the definition of the $\ell_p(L_q)$-norm, we have

$$\begin{aligned}\|f\|_{\ell_p(L_q)} \leq \|f\|_{\ell_p(L_\infty)} = \Big(\sum_{\mathbf{n}\in\mathbb{Z}^d} \|f\chi_{\mathscr{Q}_{\mathbf{n}}}\|_\infty^p\Big)^{\frac{1}{p}} &\overset{(2.19)}{\leq} \mathrm{const} \cdot \Big(\sum_{\boldsymbol{\alpha}\in\{0,1\}^d} \sum_{\mathbf{n}\in\mathbb{Z}^d} \big\|(\nabla^{\boldsymbol{\alpha}} f)\chi_{\mathscr{Q}_{\mathbf{n}}}\big\|_p^p\Big)^{\frac{1}{p}} \\ &= \mathrm{const} \cdot \Big(\sum_{\alpha\in\{0,1\}^d} \|\nabla^{\boldsymbol{\alpha}} f\|_p^p\Big)^{\frac{1}{p}}.\end{aligned}$$

Additionally, since ℓ_1 is nested within ℓ_p, we observe that

$$\Big(\sum_{\boldsymbol{\alpha}\in\{0,1\}^d} \|\nabla^{\boldsymbol{\alpha}} f\|_p^p\Big)^{\frac{1}{p}} \leq \sum_{\boldsymbol{\alpha}\in\{0,1\}^d} \|\nabla^{\boldsymbol{\alpha}} f\|_p.$$

Hence, for all $f \in W_p^d(\mathbb{R}^d) \cap C_{\mathrm{b}}^d(\mathbb{R}^d)$, we have the estimate

$$\|f\|_{\ell_p(L_q)} \leq \mathrm{const} \cdot \sum_{\boldsymbol{\alpha}\in\{0,1\}^d} \|\nabla^{\boldsymbol{\alpha}} f\|_p \leq \mathrm{const} \cdot \|f\|_{W_p^d}.$$

Therefore, since $W_p^d(\mathbb{R}^d) \cap C_{\mathrm{b}}^d(\mathbb{R}^d)$ is dense in $W_p^d(\mathbb{R}^d)$, we conclude that

$$\|f\|_{\ell_p(L_q)} \leq \mathrm{const} \cdot \|f\|_{W_p^d}, \quad \text{for all } f \in W_p^d(\mathbb{R}^d). \qquad \square$$

We state the following special case of the Cwikel estimates for weak Schatten ideals, which we shall make use of in both Chapters 3 and 4 below.

Proposition 2.56. *Let $1 \leq p < \infty$, and suppose that $\delta \geq \frac{d}{p}$.*

(*i*) *Suppose $2 < p < \infty$. If $f \in L_p(\mathbb{R}^d)$, then $M_f \langle\nabla\rangle^{-\delta} \in \mathcal{L}_{p,\infty}$.*

(*ii*) *Suppose $1 \leq p < 2$. If $f \in W_p^d(\mathbb{R}^d)$, then $M_f \langle\nabla\rangle^{-\delta} \in \mathcal{L}_{p,\infty}$.*

(*iii*) *Suppose $p = 2$. If $f \in W_2^d(\mathbb{R}^d)$, then $M_f \langle\nabla\rangle^{-2\delta} \in \mathcal{L}_{2,\infty}$.*

Proof. (i). Let $p > 2$, and suppose $f \in L_p(\mathbb{R}^d)$. By Theorem 2.46, we have that $M_f\langle\nabla\rangle^{-\delta} \in \mathcal{L}_{p,\infty}$ for all $\delta \geq \frac{d}{p}$, since $\langle\cdot\rangle^{-\delta} \in L_{p,\infty}(\mathbb{R}^d)$ for all $\delta \geq \frac{d}{p}$.

(ii). Let $1 \leq p < 2$, and suppose $f \in W_p^d(\mathbb{R}^d)$. By Remark 2.51, we have that $\langle\cdot\rangle^{-\delta} \in \ell_{p,\infty}(L_2)(\mathbb{R}^d)$, for all $\delta \geq \frac{d}{p}$. Hence, by Theorem 2.52, we have that $M_f\langle\nabla\rangle^{-\delta} \in \mathcal{L}_{p,\infty}$, for all $\delta \geq \frac{d}{p}$.

(iii). Let $p = 2$, and suppose $f \in W_2^d(\mathbb{R}^d)$. By (ii), we have that $M_{|f|^2}\langle\nabla\rangle^{-2\delta} \in \mathcal{L}_{1,\infty}$, since $|f|^2 \in W_1^d(\mathbb{R}^d)$ by the Leibniz rule. Therefore, by [78, Theorem 3.1], we have that

$$\left\|M_f\langle\nabla\rangle^{-\delta}\right\|_{2,\infty} = \left\|\langle\nabla\rangle^{-\delta}M_{|f|^2}\langle\nabla\rangle^{-\delta}\right\|_{1,\infty}^{\frac{1}{2}} \leq \|M_{|f|^2}\langle\nabla\rangle^{-2\delta}\|_{1,\infty}^{\frac{1}{2}} < \infty,$$

so $M_f\langle\nabla\rangle^{-\delta} \in \mathcal{L}_{2,\infty}$. □

2.6 Operator integration

In this section, we introduce one of the main technical tools of the thesis: double operator integrals.

2.6.1 Weak operator integration

The foundation of double operator integrals in this text is based upon the following notion of the weak operator integral. The exposition in this section closely follows Section 2.7 of [25]. We assume throughout that (Ω, ν) is a σ-finite measure space.

Definition 2.57. Let $f : \Omega \to \mathcal{B}(\mathcal{H})$ be a function. Such a function is *weak operator ν-measurable* if, for all $\xi, \eta \in \mathcal{H}$, the map

$$\omega \mapsto \langle f(\omega)\xi, \eta\rangle, \quad \omega \in \Omega,$$

is ν-measurable.

Definition 2.58. Suppose $f : \Omega \to \mathcal{B}(\mathcal{H})$ is weak operator ν-measurable. We say that f is *weak operator ν-integrable* if

$$\int_\Omega \left\|f(\omega)\right\|_\infty \mathrm{d}\nu(\omega) < \infty. \tag{2.20}$$

Now, define a sesquilinear form

$$(\xi, \eta)_f := \int_\Omega \langle f(\omega)\xi, \eta\rangle \,\mathrm{d}\nu(\omega), \quad \text{for } \xi, \eta \in \mathcal{H},$$

from which we see that

$$\left|(\xi, \eta)_f\right| \leq \Big(\int_\Omega \left\|f(\omega)\right\|_\infty \mathrm{d}\nu(\omega)\Big)\|\xi\|\|\eta\|, \quad \text{for } \xi, \eta \in \mathcal{H}.$$

Hence, fixing $\xi \in \mathcal{H}$, the map $\eta \mapsto (\xi, \eta)_f$ defines a bounded, anti-linear functional on $\mathcal{H}$. Hence, by the Riesz representation theorem, there exists an element, which we shall denote by $\int_\Omega f(\omega)\xi \,\mathrm{d}\nu(\omega) \in \mathcal{H}$, such that

$$\Big\langle \int_\Omega f(\omega)\xi \,\mathrm{d}\nu(\omega), \eta \Big\rangle := (\xi, \eta)_f = \int_\Omega \langle f(\omega)\xi, \eta\rangle \,\mathrm{d}\nu(\omega), \quad \text{for all } \eta \in \mathcal{H}.$$

Definition 2.59. Suppose $f : \Omega \to \mathcal{B}(\mathcal{H})$ is weak operator ν-integrable. The *weak operator integral* of f is the operator defined by the expression

$$\Big(\int_\Omega f(\omega) \,\mathrm{d}\nu(\omega) \Big)\xi := \int_\Omega f(\omega)\xi \,\mathrm{d}\nu(\omega), \quad \text{for } \xi \in \mathcal{H}.$$

Remark 2.60. By construction, we have that

$$\Big\| \int_\Omega f(\omega) \,\mathrm{d}\nu(\omega) \Big\|_\infty \leq \int_\Omega \big\| f(\omega) \big\|_\infty \,\mathrm{d}\nu(\omega). \tag{2.21}$$

The following result is well-known for Bochner integrals. For the case of weak operator integrals, we refer the reader to, e.g., [87, Lemma 2.3.2].

Lemma 2.61. *Suppose $\Omega \subset \mathbb{R}^d$ is a measurable subset of the plane, for some $d \in \mathbb{Z}_+$, and suppose $f : \Omega \to \mathcal{B}(\mathcal{H})$ is continuous in the weak operator topology. If $f(x) \in \mathcal{L}_1(\mathcal{H})$, for all $x \in \Omega$, and if*

$$\int_\Omega \big\| f(t) \big\|_1 \,\mathrm{d}t < \infty,$$

then f is ν-integrable in the weak operator topology, $\int_\Omega f(t)\,\mathrm{d}t \in \mathcal{L}_1(\mathcal{H})$ and

$$\Big\| \int_\Omega f(t) \,\mathrm{d}t \Big\|_1 \leq \int_\Omega \big\| f(t) \big\|_1 \,\mathrm{d}t. \tag{2.22}$$

2.6.2 Double operator integration

Double operator integrals are used to obtain Lipschitz-type estimates and commutator estimates that shall be used in both Chapters 3 and 4 below. First appearing in the work of Yu. Daleckiĭ and S. Kreĭn [28, 29], double operator integrals were thoroughly treated in the setting of $\mathcal{K}(\mathcal{H})$ by M. Birman and M. Solomyak [8, 9, 11] (see the survey [13] for further details) and have been extensively developed in recent years [61, 59, 63, 60, 65, 66, 67].

Suppose X, Y are self-adjoint operators on a separable Hilbert space $\mathcal{H}$, and h is a bounded, Borel-measurable function on $\sigma(X) \times \sigma(Y) \subset \mathbb{R}^2$. Heuristically, the double operator integral $\mathcal{J}_h^{X,Y}$ is then defined as an operator on $\mathcal{L}_2$ expressed in terms of the product of the spectral measures of X, Y by

$$\mathcal{J}_h^{X,Y} = \int_{\sigma(Y)} \int_{\sigma(X)} h(\lambda, \mu) \,\mathrm{d}(\mathsf{E}_X \otimes \mathsf{E}_Y)(\lambda, \mu). \tag{2.23}$$

To ensure that this construction defines a bounded operator on the other Schatten–von Neumann classes, we require that the function h belong to the integral projective tensor product (see, e.g., [63]).

Definition 2.62. Suppose X, Y be self-adjoint operators on $\mathcal{H}$. Let h be a bounded, Borel-measurable function on $\sigma(X) \times \sigma(Y)$. If there exists a σ-finite measure space (Ω, ν) and Borel $(\mathsf{m} \times \nu)$-measurable functions h_1, h_2 on $\sigma(X) \times \Omega$, $\sigma(Y) \times \Omega$, respectively (where m denotes the Lebesgue measure on $\sigma(X), \sigma(Y) \subset \mathbb{R}$), satisfying the conditions

$$\int_\Omega \Big(\sup_{\lambda \in \sigma(X)} \big|h_1(\lambda, \omega)\big| \Big) \Big(\sup_{\mu \in \sigma(Y)} \big|h_2(\mu, \omega)\big| \Big) \, \mathrm{d}\nu(\omega) < \infty, \tag{2.24}$$

and

$$h(\lambda, \mu) = \int_\Omega h_1(\lambda, \omega) h_2(\mu, t) \, \mathrm{d}\nu(\omega), \quad \text{for } \lambda \in \sigma(X),\ \mu \in \sigma(Y), \tag{2.25}$$

then h is said to belong to the *integral projective tensor product* of X and Y, denoted $\mathfrak{A}_{X,Y}$.

This function space forms a Banach algebra under the norm

$$\|h\|_{\mathfrak{A}_{X,Y}} := \inf_{h_1, h_2} \int_\Omega \Big(\sup_{\lambda \in \sigma(X)} \big|h_1(\lambda, \omega)\big| \Big) \Big(\sup_{\mu \in \sigma(Y)} \big|h_2(\mu, \omega)\big| \Big) \, \mathrm{d}\nu(\omega), \quad \text{for } h \in \mathfrak{A}_{X,Y},$$

where the above infimum runs over all possible choices of h_1, h_2 satisfying (2.24), (2.25) (see [59] for details).

Suppose $\mathcal{A} \in \mathcal{B}(\mathcal{H})$. By construction, if $h \in \mathfrak{A}_{X,Y}$ and h_1, h_2 are Borel functions satisfying (2.24) and (2.25) for h, then the function

$$\omega \mapsto \big\langle h_1(X, \omega) A h_2(Y, \omega) \xi, \eta \big\rangle, \quad \omega \in \Omega,$$

is ν-measurable, for all $\xi, \eta \in \mathcal{H}$. Combining this with (2.24), we see that the map $\omega \mapsto h_1(X, \omega) A h_2(Y, \omega)$ is weak operator ν-integrable.

Definition 2.63. Suppose X, Y are self-adjoint operators on $\mathcal{H}$, and suppose $h \in \mathfrak{A}_{X,Y}$. The *double operator integral (DOI)* $\mathcal{J}_h^{X,Y}$ is the operator on $\mathcal{B}(\mathcal{H})$ defined by the expression

$$\mathcal{J}_h^{X,Y}(A) := \int_\Omega h_1(X, \omega) A h_2(Y, \omega) \, \mathrm{d}\nu(\omega), \quad \text{for } A \in \mathcal{B}(\mathcal{H}), \tag{2.26}$$

where h_1, h_2 are any Borel functions satisfying (2.24) and (2.25) for h, the operators $h_1(X, \omega)$ and $h_2(Y, \omega)$ are understood via the Borel functional calculus for each $\omega \in \Omega$, and the integral over Ω is understood as a weak operator integral (as in Definition 2.59 above).

Proposition 2.64. [59, Proposition 4.7], [66, Corollary 2] *If X, Y are self-adjoint operators on $\mathcal{H}$, $h \in \mathfrak{A}_{X,Y}$, and $1 \leq p \leq \infty$, then $\mathcal{J}_h^{X,Y}$ is bounded on $\mathcal{L}_p(\mathcal{H})$, and*

$$\|\mathcal{J}_h^{X,Y}\|_{p\to p} \leq \|h\|_{\mathfrak{A}_{X,Y}}, \tag{2.27}$$

where $\|\cdot\|_{p\to p}$ denotes the uniform norm for operators on $\mathcal{L}_p$.

The properties of double operator integrals have been used to prove Lipschitz estimates for $\mathcal{L}_p$ (for functions belonging to the Besov space $B^1_{\infty,1}(\mathbb{R})$ when $p = 1$ [62, Theorem 4], and for Lipschitz functions when $1 < p < \infty$ [67, Theorem 1]). Theorems 2.66 and 2.65 below shall suffice for our purposes.

Suppose $h \in C^1(\mathbb{R})$. We define the *divided difference* of h by the expression

$$h^{[1]}(x,y) = \begin{cases} \dfrac{h(x)-h(y)}{x-y}, & \text{if } x \neq y, \\ h'(x), & \text{if } x = y, \end{cases} \qquad x, y \in \mathbb{R},$$

where h' denotes the derivative of h. We seek sufficient conditions on h for the divided difference $h^{[1]}$ to belong to the integral projective tensor product $\mathfrak{A}_{X,Y}$ for any self-adjoint X, Y.

Theorem 2.65. [66, Theorem 4] *Suppose X, Y are self-adjoint operators on $\mathcal{H}$. If $h \in C^2_{\mathrm{b}}(\mathbb{R})$, then $h^{[1]} \in \mathfrak{A}_{X,Y}$ and*

$$\|h^{[1]}\|_{\mathfrak{A}_{X,Y}} \leq \mathrm{const} \cdot \big(\|h\|_\infty + \|h'\|_\infty + \|h''\|_\infty\big).$$

The following result was originally stated in the more general setting of semifinite von Neumann algebras, and for a more general family of functions belonging to the integral projective tensor product.

Theorem 2.66. [65, Theorem 3.1] *Suppose X, Y are self-adjoint operators on $\mathcal{H}$ with a common core $\mathcal{C} \subset \mathcal{H}$, and $A \in \mathcal{B}(\mathcal{H})$, such that $A(\mathcal{C}) \subset \mathcal{C}$ and $XA - AY$, defined initially on $\mathcal{C}$, has bounded extension. If $h \in C^2_{\mathrm{b}}(\mathbb{R})$, then $h(X)A - Ah(Y) \in \mathcal{B}(\mathcal{H})$ and*

$$h(X)A - Ah(Y) = \mathcal{J}^{X,Y}_{h^{[1]}}(XA - AY). \tag{2.28}$$

Additionally, if $XA - AY \in \mathcal{L}_p(\mathcal{H})$, then $h(X)A - Ah(Y) \in \mathcal{L}_p(\mathcal{H})$ and

$$\begin{aligned} \big\|h(X)A - Ah(Y)\big\|_p &\leq \|\mathcal{J}^{X,Y}_{h^{[1]}}\|_{p\to p}\|XA - AY\|_p \\ &\leq \mathrm{const} \cdot \big(\|h\|_\infty + \|h'\|_\infty + \|h''\|_\infty\big) \cdot \|XA - AY\|_p. \end{aligned} \tag{2.29}$$

Note that the second line of (2.29) follows from (2.27) and Theorem 2.65.

In Section 3.3.2 below, we shall want a Lipschitz estimate similar to the above theorem, but for possibly unbounded $h \in \mathfrak{A}_{X,Y}$. To this end, we shall use estimate for the L_1-norm of a Fourier transform of a continuous square-integrable function.

Lemma 2.67. [66, Lemma 7] *Suppose $f \in L_2(\mathbb{R}) \cap C^1(\mathbb{R})$. If $f' := \frac{\mathrm{d}f}{\mathrm{d}x} \in L_2(\mathbb{R})$, then $\mathcal{F}(f) \in L_1(\mathbb{R})$ and*

$$\big\|\mathcal{F}(f)\big\|_1 \leq \sqrt{2}\big(\|f\|_2 + \|f'\|_2\big). \tag{2.30}$$

We provide the proof of the following lemma below for the convenience of the reader.

Lemma 2.68. [89, Lemma 2.8] *Suppose B is a self-adjoint operator on $\mathcal{H}$. If $h \in C^2(\mathbb{R})$ such that $h' \in W_2^1(\mathbb{R})$, then $h^{[1]} \in \mathfrak{A}_{B,B}$ and*

$$\|h^{[1]}\|_{\mathfrak{A}_{B,B}} \leq \sqrt{2}\big(\|h'\|_2 + \|h''\|_2\big).$$

Proof. By Fourier inversion [69, Theorem IX.1] on h', the divided difference $h^{[1]}$ of h may be expressed as

$$h^{[1]}(x,y) = \int_0^1 h'\big(sx + (1-s)y\big)\,\mathrm{d}s = \frac{1}{\sqrt{2\pi}} \int_0^1 \int_{\mathbb{R}} \widehat{(h')}(t) e^{it(sx+(1-s)y)}\,\mathrm{d}t\,\mathrm{d}s.$$

Observe that we may construct functions $h_1, h_2 : \mathbb{R} \times \big([0,1] \times \mathbb{R}\big) \to \mathbb{C}$ defined by

$$h_1\big(x,(s,t)\big) := e^{itsx}, \quad h_2\big(y,(s,t)\big) := e^{it(1-s)y},$$

and a measure ν on $[0,1] \times \mathbb{R}$ given by $\mathrm{d}\nu(s,t) := \widehat{(h')}(t)\,\mathrm{d}t\,\mathrm{d}s$ such that the decomposition

$$h^{[1]}(x,y) = \frac{1}{\sqrt{2\pi}} \int_{[0,1]\times\mathbb{R}} h_1\big(x,(s,t)\big) h_2\big(y,(s,t)\big)\,\mathrm{d}\nu(s,t). \tag{2.31}$$

However, appealing to Lemma 2.67 above, since $h' \in C^1(\mathbb{R})$ and $h', h'' \in L_2(\mathbb{R})$ by assumption, we have that $\widehat{(h')} \in L_1(\mathbb{R})$ and

$$\big\|\widehat{(h')}\big\|_1 \leq \sqrt{2}\big(\|h'\|_2 + \|h''\|_2\big).$$

Hence, the decomposition (2.31) satisfies (2.24) and (2.25), and $h^{[1]} \in \mathfrak{A}_{B,B}$, with

$$\|h^{[1]}\|_{\mathfrak{A}_{B,B}} \leq \big\|\widehat{(h')}\big\|_1.$$

□

Theorem 2.69. [65, Theorem 5.3] *Let $p \geq 1$. Suppose $A \in \mathcal{B}(\mathcal{H})$ and B is a self-adjoint operator on $\mathcal{H}$ such that $A\big(\mathrm{dom}(B)\big) \subset \mathrm{dom}(B)$ and $[A,B] \in \mathcal{L}_p(\mathcal{H})$. If $h \in C^2(\mathbb{R})$ such that $h' \in W_2^1(\mathbb{R})$, then*

$$\Big\|\big[A, h(B)\big]\Big\|_p \leq \mathrm{const} \cdot \big(\|h'\|_2 + \|h''\|_2\big) \cdot \big\|[A,B]\big\|_p.$$

3

Zeta residues

The contents of this chapter are the product of my work with co-authors in [68]. We prove the zeta residue formula stated in Theorem 1.1. We then proceed to use this result to provide alternative proofs for Connes' integral formula for $\mathbb{R}^d$ [48] and the Moyal plane [86].

3.1 Concerning a lemma of Connes

In [24, Lemma 11 (§IV.3.α)], A. Connes stated

Conjecture 3.1. *Let $p > 1$, and let $\mathcal{H} = L_2(\mathbb{S}^1)$. If $0 \leq f \in L_\infty(\mathbb{S}^1)$, and $0 \leq B \in \mathcal{L}_{p,\infty}\big(L_2(\mathbb{S}^1)\big)$ such that $[M_f, B] \in \Big(\mathcal{L}_{p,\infty}\big(L_2(\mathbb{S}^1)\big)\Big)_0$, then*

$$M_f^{\frac{p}{2}} B^p M_f^{\frac{p}{2}} - (M_f^{\frac{1}{2}} B M_f^{\frac{1}{2}})^p \in \Big(\mathcal{L}_{1,\infty}\big(L_2(\mathbb{S}^1)\big)\Big)_0.$$

Combining with Theorem 1.5, Conjecture 3.1 states that $M_f^{\frac{1}{2}} B M_f^{\frac{1}{2}} \in \mathcal{M}_{1,\infty}$ and

$$\mathrm{Tr}_\omega(M_f^{\frac{1}{2}} B M_f^{\frac{1}{2}}) = \lim_{p\downarrow 1}(p-1)\,\mathrm{Tr}(M_f^{\frac{p}{2}} B^p M_f^{\frac{p}{2}})$$

whenever the limit on the right-hand side exists. This later limit is often easier to find, which is the utility of this conjecture.

A variant of Conjecture 3.1 was recently proved in [25] by A. Connes, F. Sukochev and D. Zanin.

Proposition 3.2. [25, Lemma 5.3] *Suppose $0 \leq A \in \mathcal{B}(\mathcal{H})$ and $0 \leq B \in \mathcal{L}_{p,\infty}$, for some $1 < p < \infty$. If $[A^{\frac{1}{2}}, B] \in (\mathcal{L}_{p,\infty})_0$, then*

$$B^p A^p - (A^{\frac{1}{2}} B A^{\frac{1}{2}})^p \in (\mathcal{L}_{1,\infty})_0.$$

The main result of this section is a trace-class version of Proposition 3.2. A significant difference is that the requirement that $B \in \mathcal{L}_{p,\infty}$ is removed.

Proposition 3.3. *If* $0 \le A, B \in \mathcal{B}(\mathcal{H})$ *such that* $[A^{\frac{1}{2}}, B] \in \mathcal{L}_1$*, then*

$$\lim_{p \downarrow 1} (p-1) \operatorname{Tr}\left(B^p A^p - (A^{\frac{1}{2}} B A^{\frac{1}{2}})^p\right) = 0. \tag{3.1}$$

The proof of Proposition 3.2 in [25] used double operator integrals to obtain a weak integral representation of the difference $B^p A^p - (A^{\frac{1}{2}} B A^{\frac{1}{2}})^p$. We shall use the same key approach to prove Proposition 3.3.

For $1 < p < 2$, we define a function g_p on $\mathbb{R}$ by setting

$$g_p(t) := \begin{cases} \dfrac{1}{2}\Big(1 - \coth\Big(\dfrac{t}{2}\Big) \tanh\Big(\dfrac{(p-1)t}{2}\Big)\Big), & \text{if } t \neq 0, \\[2ex] 1 - \dfrac{p}{2}, & \text{if } t = 0. \end{cases}$$

Lemma 3.4. [87, Remark 5.2.2] *For all* $1 < p < \infty$*, the function* $g_p \in \mathcal{S}(\mathbb{R})$.

Proof. Observe that, for each $1 < p < \infty$, the function g_p is even. Moreover, g_p and all of its derivatives are bounded and smooth within a neighbourhood of zero (see Lemma A.1 and its proof in the appendix). Therefore, since coth and tanh are also smooth and bounded away from zero, we have that $g_p \in C_{\mathrm{b}}^{\infty}(\mathbb{R})$. Hence, since g_p is even, it suffices to show that g_p is rapidly decreasing as $t \to \infty$.

By the definitions of the hyperbolic functions, we have the expression

$$\begin{aligned} g_p(t) &= \frac{1}{2}\Big(1 - \frac{(e^t+1)(e^{(p-1)t}-1)}{(e^t-1)(e^{(p-1)t}+1)}\Big) \\ &= \frac{e^{2t} - e^{pt}}{(e^t-1)(e^t+e^{pt})} \sim e^{(1-p)t}, \quad \text{as } t \to \infty. \end{aligned}$$

In a similar fashion, all derivatives of g_p have exponential decay at $t \to \infty$. However, polynomial growth is dominated by exponential decay; that is,

$$t^n g_p(t) \sim t^n e^{(1-p)t} = o(e^{\frac{(1-p)t}{2}}), \quad \text{as } t \to \infty.$$

Hence, we conclude that g_p is a Schwartz function. $\square$

Proposition 3.2 is proved in [25] using the following decomposition lemma. For brevity, if $0 \le A, B \in \mathcal{B}(\mathcal{H})$, then we let

$$Y = Y(A, B) := A^{\frac{1}{2}} B A^{\frac{1}{2}} \tag{3.2}$$

Additionally, for $1 < p < \infty$, define the family of operators

$$T_0 := B^{p-1}[B, A^p] + B^{p-1}A^{p-\frac{1}{2}}[A^{\frac{1}{2}}, B] + [B, A]Y^{p-1} + A^{\frac{1}{2}}[A^{\frac{1}{2}}, B]Y^{p-1}, \tag{3.3}$$

$$\begin{aligned} T_s := {} & B^{p-1+is}[B, A^{p+is}]Y^{-is} + B^{p-1+is}A^{p-\frac{1}{2}+is}[A^{\frac{1}{2}}, B]Y^{-is} \\ & + B^{is}[B, A^{1+is}]Y^{p-1-is} + B^{is}A^{\frac{1}{2}+is}[A^{\frac{1}{2}}, B]Y^{p-1-is}, \quad s \in \mathbb{R} \setminus \{0\}. \end{aligned} \tag{3.4}$$

Lemma 3.5. [87, Theorem 5.2.1] *Let $0 \le A, B \in \mathcal{B}(\mathcal{H})$. If $1 < p < \infty$, then*

$$B^p A^p - (A^{\frac{1}{2}} B A^{\frac{1}{2}})^p = T_0 - \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{g}_p(s) T_s \, \mathrm{d}s, \tag{3.5}$$

where the integral may be understood in the weak sense of Definition 2.58.

These complicated formulas for T_s, $s \ge 0$, are the product of technical computations using double operator integral representations of differences of operators. The key observation is that if X, Y are positive operators, then one can show that

$$\mathcal{J}_{\phi_1}^{X,Y}\big(X^{p-1}(X-Y)+(X-Y)Y^{p-1}\big) = \mathcal{J}_{\phi_2}^{X,Y}(1) = X^{p-1}(X-Y)+(X-Y)Y^{p-1}-(X^p-Y^p),$$

where

$$\phi_1(\lambda, \mu) := \begin{cases} g_p\Big(\log\big(\dfrac{\lambda}{\mu}\big)\Big), & \text{if } \lambda \neq 0 \text{ and } \mu \neq 0, \\ 0, & \text{otherwise,} \end{cases}$$

$$\phi_2(\lambda, \mu) := (\lambda^{p-1} + \mu^{p-1})(\lambda - \mu) - (\lambda^p - \mu^p), \qquad \text{for } \lambda, \mu \ge 0.$$

The reader is referred to [25, §5] and [87, §5.2] for the full details.

We shall use this integral decomposition to show that the trace of the difference $(p-1)\big(B^p A^p - (A^{\frac{1}{2}} B A^{\frac{1}{2}})^p\big)$ is $o(1)$ as $p \downarrow 1$, whenever $[A^{\frac{1}{2}}, B]$ is trace-class.

Proof of Proposition 3.3.

Firstly, we define the following operators for brevity:

$$X_1 := \int_{\mathbb{R}} \hat{g}_p(s) B^{is}[B, A^{p+is}]Y^{-is} \, \mathrm{d}s, \qquad X_2 := \int_{\mathbb{R}} \hat{g}_p(s) B^{is} A^{p-\frac{1}{2}+is}[A^{\frac{1}{2}}, B]Y^{-is} \, \mathrm{d}s,$$

$$X_3 := \int_{\mathbb{R}} \hat{g}_p(s) B^{is}[B, A^{1+is}]Y^{-is} \, \mathrm{d}s, \qquad X_4 := \int_{\mathbb{R}} \hat{g}_p(s) B^{is} A^{\frac{1}{2}+is}[A^{\frac{1}{2}}, B]Y^{-is} \, \mathrm{d}s.$$

Then, appealing to Lemma 3.5, we have the decomposition

$$\begin{aligned} B^p A^p - Y^p & \overset{(3.5)}{=} T_0 - \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{g}_p(s) T_s \, \mathrm{d}s \\ & = T_0 - (2\pi)^{-\frac{1}{2}} B^{p-1}(X_1 + X_2) - (2\pi)^{-\frac{1}{2}}(X_3 + X_4)Y^{p-1}. \end{aligned} \tag{3.6}$$

We treat only the term $B^{p-1}X_1$; the other terms may be considered using similar arguments. Consider the function $q_{p,s}$ defined by the expression

$$q_{p,s}(x) := \begin{cases} x^{2(p+is)}\psi_A(x), & \text{if } x \in \mathbb{R}\setminus\{0\}, \\ 0, & \text{if } x = 0. \end{cases}$$

where ψ_A is any function belonging to $C^2_{\text{com}}(\mathbb{R})$ such that $\|\psi_A\|_\infty, \|\psi_A'\|_\infty, \|\psi_A''\|_\infty \le 1$ and $\psi_A(x) = 1$, for all $x \in \big[0, \|A\|_\infty\big]$. Then, since $p > 1$, we also have that $q_{p,s} \in C^2_{\text{com}}(\mathbb{R})$. By Theorem 2.66, we have that

$$\begin{aligned} \big\|[B, A^{p+is}]\big\|_1 &\overset{(2.29)}{\le} \text{const} \cdot \big(\|q_{p,s}\|_\infty + \|q_{p,s}'\|_\infty + \|q_{p,s}''\|_\infty\big)\big\|[B, A^{\frac12}]\big\|_1 \\ &\le \begin{cases} \mathcal{O}(1)\cdot \big\|[B, A^{\frac12}]\big\|_1, & \text{if } |s| \le 1 \\ \mathcal{O}(s^2)\cdot \big\|[B, A^{\frac12}]\big\|_1, & \text{if } |s| > 1. \end{cases} \end{aligned}$$

However, this gives us the estimate

$$\begin{aligned} \int_{\mathbb{R}} \big|\hat{g}_p(s)\big|\big\|B^{is}[B, A^{p+is}]Y^{-is}\big\|_1\,\mathrm{d}s &\le \int_{\mathbb{R}} \big|\hat{g}_p(s)\big|\big\|[B, A^{p+is}]\big\|_1\,\mathrm{d}s \\ &\le \text{const}\cdot \int_{\mathbb{R}} (1+s^2)\big|\hat{g}_p(s)\big|\big\|[B, A^{\frac12}]\big\|_1\,\mathrm{d}s \\ &= \text{const}\cdot \big(\|\hat{g}_p\|_1 + \|\widehat{g_p''}\|_1\big)\big\|[B, A^{\frac12}]\big\|_1 \\ &\overset{(2.30)}{\le} \text{const}\cdot \big(\|g_p\|_2 + \|g_p'\|_2 + \|g_p''\|_2 + \|g_p'''\|_2\big)\big\|[B, A^{\frac12}]\big\|_1, \end{aligned} \tag{3.7}$$

where the second last line follows from the duality of differentiation and multiplication by a polynomial under the Fourier transform, and the last line follows from Lemma 2.67, since $g_p, g_p'' \in \mathcal{S}(\mathbb{R})$. Therefore, appealing to Lemma 2.61, we obtain

$$\begin{aligned} \|X_1\|_1 &\overset{(2.22)}{\le} \int_{\mathbb{R}} \big|\hat{g}_p(s)\big|\big\|B^{is}[B, A^{p+is}]Y^{-is}\big\|_1\,\mathrm{d}s \\ &\overset{(3.7)}{\le} \text{const}\cdot \big(\|g_p\|_2 + \|g_p'\|_2 + \|g_p''\|_2 + \|g_p'''\|_2\big)\big\|[B, A^{\frac12}]\big\|_1. \end{aligned}$$

Hence, by Lemma A.3 (see Appendix A.1 below), we have the estimate

$$\big|(p-1)\,\mathrm{Tr}(B^{p-1}X_1)\big| \le (p-1)\|B^{p-1}\|_\infty\|X_1\|_1 \le \mathcal{O}\big((p-1)^{\frac12}\big), \quad p \downarrow 1.$$

Repeating this argument for the remaining terms on the right-hand side of (3.6), we obtain the estimate

$$\big|(p-1)\,\mathrm{Tr}(B^pA^p - Y^p)\big| \le \mathcal{O}\big((p-1)^{\frac12}\big). \qquad \square$$

3.2 A locally compact residue formula

In this section, we prove one of the main results of this thesis, Theorem 1.1. Appealing to Proposition 3.3, we obtain the following result for $\mathcal{M}_{1,\infty}$.

Theorem 3.6. *Suppose $0 \leq A, B \in \mathcal{B}(\mathcal{H})$ are such that $AB \in \mathcal{M}_{1,\infty}$. Suppose that $[A^{\frac{1}{2}}, B] \in \mathcal{L}_1$. Let $C \geq 0$ be some real number. The following are equivalent:*

(i) AB is Dixmier measurable, and $\mathrm{Tr}_\omega(AB) = C$ for all dilation-invariant extended limits ω.

(ii) $\lim_{\varepsilon\downarrow 0} \varepsilon \,\mathrm{Tr}(B^{1+\varepsilon}A^{1+\varepsilon}) = C$.

Proof. Firstly, since $[A^{\frac{1}{2}}, B] \in \mathcal{L}_1(\mathcal{H})$ and $AB \in \mathcal{M}_{1,\infty}(\mathcal{H})$ by assumption, we have that $A^{\frac{1}{2}}BA^{\frac{1}{2}} = BA + [A^{\frac{1}{2}}, B]A^{\frac{1}{2}} \in \mathcal{M}_{1,\infty}(\mathcal{H})$ and

$$\mathrm{Tr}_\omega(AB) = \mathrm{Tr}_\omega(A^{\frac{1}{2}}BA^{\frac{1}{2}}) + \mathrm{Tr}_\omega\left([A^{\frac{1}{2}}, B]A^{\frac{1}{2}}\right) = \mathrm{Tr}_\omega(A^{\frac{1}{2}}BA^{\frac{1}{2}}).$$

First, we show that $(ii) \Rightarrow (i)$. Assume that the limit $\lim_{\varepsilon\downarrow 0} \varepsilon \,\mathrm{Tr}(B^{1+\varepsilon}A^{1+\varepsilon})$ exists. Then, we have by Proposition 3.3 that the limit $\lim_{\varepsilon\downarrow 0} \varepsilon \,\mathrm{Tr}\left((A^{\frac{1}{2}}BA^{\frac{1}{2}})^{1+\varepsilon}\right)$ exists and agrees with the former. Hence, appealing to Theorem 1.5 above,

$$\mathrm{Tr}_\omega(A^{\frac{1}{2}}BA^{\frac{1}{2}}) = \lim_{\varepsilon\downarrow 0} \varepsilon \,\mathrm{Tr}\left((A^{\frac{1}{2}}BA^{\frac{1}{2}})^{1+\varepsilon}\right) = \lim_{\varepsilon\downarrow 0} \varepsilon \,\mathrm{Tr}(B^{1+\varepsilon}A^{1+\varepsilon}).$$

Next, we show that $(i) \Rightarrow (ii)$. Assume that AB is Dixmier measurable. Then, again appealing to Theorem 1.5, we have that the limit $\lim_{\varepsilon\downarrow 0} \varepsilon \,\mathrm{Tr}\left((A^{\frac{1}{2}}BA^{\frac{1}{2}})^{1+\varepsilon}\right)$ exists and agrees with $\mathrm{Tr}_\omega(A^{\frac{1}{2}}BA^{\frac{1}{2}})$. Hence, by Proposition 3.3, the limit $\lim_{\varepsilon\downarrow 0} \varepsilon \,\mathrm{Tr}(B^{1+\varepsilon}A^{1+\varepsilon})$ exists and

$$\lim_{\varepsilon\downarrow 0} \varepsilon \,\mathrm{Tr}(B^{1+\varepsilon}A^{1+\varepsilon}) = \lim_{\varepsilon\downarrow 0} \varepsilon \,\mathrm{Tr}\left((A^{\frac{1}{2}}BA^{\frac{1}{2}})^{1+\varepsilon}\right) = \mathrm{Tr}_\omega(A^{\frac{1}{2}}BA^{\frac{1}{2}}). \qquad \square$$

From this result and Theorem 2.39 (see Section 2.4.2 above, which implies that, for every extended limit ω, there exists a dilation-invariant extended limit ω_0 such that, if $A \in \mathcal{L}_{1,\infty}$, then $\mathrm{Tr}_\omega(A) = \mathrm{Tr}_{\omega_0}(A)$), the result for $\mathcal{L}_{1,\infty}$ follows easily:

Theorem 3.7. *Suppose $0 \leq A, B \in \mathcal{B}(\mathcal{H})$ are such that $AB \in \mathcal{L}_{1,\infty}$. Suppose that $[A^{\frac{1}{2}}, B] \in \mathcal{L}_1$. Let $C > 0$ be some real number. The following are equivalent:*

(i) AB is Dixmier measurable, and $\mathrm{Tr}_\omega(AB) = C$ for all extended limits ω.

(ii) $\lim_{\varepsilon\downarrow 0} \varepsilon \,\mathrm{Tr}(B^{1+\varepsilon}A^{1+\varepsilon}) = C$.

Combining Theorem 3.6 with Theorem 3.7 gives Theorem 1.1.

3.3 Connes integration formula for $\mathbb{R}^d$

In this section, we calculate the Dixmier trace of the operator

$$(\mathbb{I} \otimes M_f)\langle\mathcal{D}\rangle^{-d} = \mathbb{I} \otimes M_f(1-\Delta)^{-\frac{d}{2}}$$

on the Hilbert space $\mathbb{C}^{N_d} \otimes L_2(\mathbb{R}^d)$ (where $N_d := 2^{\lfloor \frac{d}{2} \rfloor}$) for $f \in W_1^d(\mathbb{R}^d)$ using Theorem 3.7. By using Cwikel estimates (see Section 2.5.2 above), we shall see that it suffices by a density argument to apply Theorem 3.7 with

$$A = \mathbb{I} \otimes M_f \quad \text{and} \quad B = \langle\mathcal{D}\rangle^{-d}$$

for $0 \leq f \in \mathcal{S}(\mathbb{R}^d)$.

We need to check that $\left[\mathbb{I} \otimes M_{f^{\frac{1}{2}}}, \langle\mathcal{D}\rangle^{-d}\right] \in \mathcal{L}_1$. The pseudodifferential calculus tells us that

$$\left[M_f, \langle\nabla\rangle^{-d}\right] = \left[M_f, (1-\Delta)^{-\frac{d}{2}}\right] \in \mathcal{L}_1,$$

for any $\mathcal{S}(\mathbb{R}^d)$. However, we note that $\mathcal{S}(\mathbb{R}^d)$ is not closed under taking positive square roots. For example, if $f(x) = x^2 e^{-x^2}$, $x \in \mathbb{R}$, then $0 \leq f \in \mathcal{S}(\mathbb{R})$ and

$$(f^{\frac{1}{2}})'(x) = \operatorname{sgn}(x)(1-x^2)e^{-\frac{x^2}{2}}, \quad x \in \mathbb{R} \setminus \{0\},$$

which is clearly discontinuous at $x = 0$. Nonetheless, the assumption $\nabla(f^{\frac{1}{2}}) \in \ell_1(L_2)(\mathbb{R}^d)^d$ is sufficient to check that $[A^{\frac{1}{2}}, B] \in \mathcal{L}_1$ in this case, and we shall show this assumption is redundant if we already have $0 \leq f \in \mathcal{S}(\mathbb{R}^d)$.

3.3.1 Square roots of Schwartz functions

We investigate the smoothness and decay of the *nonnegative* function $f^{\frac{1}{2}} = \left|\sqrt{f}\right|$, for $0 \leq f \in \mathcal{S}(\mathbb{R}^d)$. Since $f^{\frac{1}{2}}$ may not be differentiable at the zeros of f, we make the following observations, starting with the Malgrange lemma for *strictly positive* f, whose proof supplied in [39, Lemma 1] is given below for the convenience of the reader.

Lemma 3.8 (Malgrange lemma). *If f is a strictly positive C_b^2-function on $\mathbb{R}$, then*

$$\left|(f^{\frac{1}{2}})'(x)\right| < \frac{\|f''\|_\infty^{\frac{1}{2}}}{\sqrt{2}}, \quad \textit{for every } x \in \mathbb{R}.$$

Proof. Firstly, fix some $x \in \mathbb{R}$ and choose some $\varepsilon > 0$. By Taylor's theorem, there exists a constant $c \in (x, x+\varepsilon)$ such that

$$0 < f(x+\varepsilon) = f(x) + \varepsilon f'(x) + \frac{\varepsilon^2}{2} f''(c) \leq f(x) + \varepsilon f'(x) + \frac{\varepsilon^2}{2}\|f''\|_\infty.$$

Observe that the expression on the right-hand side is a strictly positive quadratic in ε. Particularly, it has no real solutions, so it has negative discriminant—that is,

$$f'(x)^2 < 2f(x)\|f''\|_\infty, \quad x \in \mathbb{R}.$$

Taking the absolute value followed by the square root of both sides of this inequality, and dividing through both sides by $2f^{\frac{1}{2}}(x)$, yields the result. $\square$

The Malgrange lemma offers us the following Lipschitz condition on the derivative of $f^{\frac{1}{2}}$, for a *nonnegative* C_{b}^2-function f.

Corollary 3.9. *If f is a nonnegative C_{b}^2-function on $\mathbb{R}$, then $f^{\frac{1}{2}}$ is Lipschitz and*

$$\left\|(f^{\frac{1}{2}})'\right\|_\infty \leq \|f''\|_\infty^{\frac{1}{2}}.$$

Proof. For every $n \geq 1$, define the function $f_n(t) = f(t) + \frac{1}{n}$, $t \in \mathbb{R}$. Since f_n is strictly positive, we may immediately apply the Malgrange lemma above to bound the Lipschitz constant of $f_n^{\frac{1}{2}}$ by

$$\left\|(f_n^{\frac{1}{2}})'\right\|_\infty \leq \|f_n''\|_\infty^{\frac{1}{2}} = \|f''\|_\infty^{\frac{1}{2}}.$$

In particular, we have the expression

$$\left|f_n^{\frac{1}{2}}(x) - f_n^{\frac{1}{2}}(y)\right| \leq \|f''\|_\infty^{\frac{1}{2}} \cdot |x-y|, \quad \text{for all } x, y \in \mathbb{R}.$$

Taking the pointwise limit of the above as $n \to \infty$ yields the result. $\square$

Remark 3.10. Suppose $f \geq 0$ is a C_{b}^2-function on $\mathbb{R}^d$. For each $j = 1, \ldots, d$, by fixing all variables x_k, for $k \neq j$, taking the partial derivative $\partial_j(f^{\frac{1}{2}})$ is the same as taking the derivative of a univariate function. Hence, by Corollary 3.9, we have that

$$\left\|\partial_j(f^{\frac{1}{2}})\right\|_\infty \leq \|\partial_j^2 f\|_\infty^{\frac{1}{2}}. \tag{3.8}$$

An immediate consequence of this remark is that $f^{\frac{1}{2}} \in W_\infty^1(\mathbb{R}^d)$ and, by the Leibniz rule and the Hölder inequality, defines a multiplication operator invariant on Bessel potential space; that is,

$$M_{f^{\frac{1}{2}}}\left(W_2^s(\mathbb{R}^d)\right) \subseteq W_2^s(\mathbb{R}^d), \quad \text{for all } 0 \leq s \leq 1.$$

Lemma 3.11. *If $0 \leq f \in \mathcal{S}(\mathbb{R}^d)$, then*

$$\partial_j(f^{\frac{1}{2}}) \in \ell_1(L_2)(\mathbb{R}^d), \quad \textit{for every } j = 1, \ldots, d.$$

Proof. Define a function g by the expression

$$g(\mathbf{t}) = \langle \mathbf{t} \rangle^{4d} f(\mathbf{t}), \quad \mathbf{t} \in \mathbb{R}^d.$$

Observe that g is also Schwartz, since f is rapidly decreasing. Then, for each $j = 1, \ldots, d$, the Leibniz rule yields

$$\partial_j(f^{\frac{1}{2}})(\mathbf{t}) = \Big(\partial_j(g^{\frac{1}{2}})(\mathbf{t}) - 2d \cdot t_j \langle \mathbf{t} \rangle^{-2} \cdot (g^{\frac{1}{2}})(\mathbf{t})\Big) \cdot \langle \mathbf{t} \rangle^{-2d}.$$

However, it follows from Remark 3.10 that the first factor on the right-hand side of the above defines a bounded function, while the function $\langle \cdot \rangle^{-2d}$ belongs to $\ell_1(L_2)(\mathbb{R}^d)$ by Remark 2.49. This concludes the proof. $\square$

We may now obtain the following Cwikel estimate for (weak) trace class in a form convenient for the Section 3.3.2 below.

Lemma 3.12. *If $\varepsilon > 0$ and $0 \leq f \in \mathcal{S}(\mathbb{R}^d)$, then*

$$M_{\partial_j(f^{\frac{1}{2}})} \langle \nabla \rangle^{-d} \in \mathcal{L}_{1,\infty} \quad \textit{and} \quad M_{\partial_j(f^{\frac{1}{2}})} \langle \nabla \rangle^{-d-\varepsilon} \in \mathcal{L}_1,$$

for every $j = 1, \ldots, d$.

Proof. By Lemma 3.11, the function $\partial_j(f^{\frac{1}{2}}) \in \ell_1(L_2)(\mathbb{R}^d)$, for all $j = 1, \ldots, d$. Combining this with Remark 2.51 and Theorem 2.52 (with $p = 1$), we get that $M_{\partial_j(f^{\frac{1}{2}})} \langle \nabla \rangle^{-d} \in \mathcal{L}_{1,\infty}$. Likewise, by Remark 2.49 and Theorem 2.50 (with $p = 1$), we have that $M_{\partial_j(f^{\frac{1}{2}})} \langle \nabla \rangle^{-d-\varepsilon} \in \mathcal{L}_1$, whenever $\varepsilon > 0$. $\square$

3.3.2 Application of residue formula to the Euclidean plane

In this section, we use Theorem 3.7 to recover Connes' trace theorem for operators of the form $M_f \langle \nabla \rangle^{-\frac{d}{2}}$ on $\mathbb{C}^{N_d} \otimes L_2(\mathbb{R}^d)$, where $f \in W_1^d(\mathbb{R}^d)$ (see Theorem 3.16 below). First, we consider the case when $f \in \mathcal{S}(\mathbb{R}^d)$ is nonnegative.

Lemma 3.13. *Suppose $0 \leq f \in \mathcal{S}(\mathbb{R}^d)$. We have the following:*

(i)

$$\big[(\mathbb{I} \otimes M_f)^{\frac{1}{2}}, \langle \mathcal{D} \rangle^{-d}\big] \in \mathcal{L}_1.$$

(ii) For every $j, k = 1, \ldots, d$,

$$\Big[(\mathbb{I} \otimes M_f)^{\frac{1}{2}}, \big(\mathbb{I} \otimes \partial_j \partial_k (-\Delta)^{-1}\big) \langle \mathcal{D} \rangle^{-d}\Big] \in \mathcal{L}_1.$$

Proof. (i). We begin by decomposing the commutator into treatable terms. Firstly, by the identity (2.2) (see Section 2.2.1 above), we obtain the expression

$$\big[(\mathbb{I}\otimes M_f)^{\frac{1}{2}}, \langle\mathcal{D}\rangle^{-d}\big] = \sum_{k=0}^{3d-1} \langle\mathcal{D}\rangle^{-\frac{k}{3}}\big[\mathbb{I}\otimes M_{f^{\frac{1}{2}}}, \langle\mathcal{D}\rangle^{-\frac{1}{3}}\big]\langle\mathcal{D}\rangle^{\frac{k+1}{3}-d}.$$

Then, appealing to Remark 3.10, we have that since $f^{\frac{1}{2}} \in W^1_\infty(\mathbb{R}^d) \subset W^{\frac{1}{3}}_\infty(\mathbb{R}^d)$, the multiplication operator $M_{f^{\frac{1}{2}}}$ is bounded on both Hilbert spaces $L_2(\mathbb{R}^d)$ and $W_2^{\frac{1}{3}}(\mathbb{R}^d)$. Therefore, since $\langle\mathcal{D}\rangle^{\frac{1}{3}} = \mathbb{I}\otimes\langle\nabla\rangle^{\frac{1}{3}}$ is well-defined in the domain $\mathbb{C}^{N_d}\otimes W_2^{\frac{1}{3}}(\mathbb{R}^d)$ by construction, and since $\langle\mathcal{D}\rangle^{-\frac{1}{3}} = \mathbb{I}\otimes\langle\nabla\rangle^{-\frac{1}{3}}$ maps $\mathbb{C}^{N_d}\otimes L_2(\mathbb{R}^d)$ into $\mathbb{C}^{N_d}\otimes W_2^{\frac{1}{3}}(\mathbb{R}^d)$, the expression

$$\big[\mathbb{I}\otimes M_{f^{\frac{1}{2}}}, \langle\mathcal{D}\rangle^{-\frac{1}{3}}\big] = -\langle\mathcal{D}\rangle^{-\frac{1}{3}}\big[\mathbb{I}\otimes M_{f^{\frac{1}{2}}}, \langle\mathcal{D}\rangle^{\frac{1}{3}}\big]\langle\mathcal{D}\rangle^{-\frac{1}{3}}$$

is well-defined on all of $\mathbb{C}^{N_d}\otimes L_2(\mathbb{R}^d)$. Therefore,

$$\begin{aligned}\big[\mathbb{I}\otimes M_{f^{\frac{1}{2}}}, \langle\mathcal{D}\rangle^{-d}\big] &= \sum_{k=0}^{3d-1}\langle\mathcal{D}\rangle^{-\frac{k+1}{3}}\big[\mathbb{I}\otimes M_{f^{\frac{1}{2}}}, \langle\mathcal{D}\rangle^{\frac{1}{3}}\big]\langle\mathcal{D}\rangle^{\frac{k}{3}-d}\\ &= -\sum_{k=0}^{3d-1}\big[\langle\mathcal{D}\rangle^{-\frac{k+1}{3}}(\mathbb{I}\otimes M_{f^{\frac{1}{2}}})\langle\mathcal{D}\rangle^{\frac{k}{3}-d}, \langle\mathcal{D}\rangle^{\frac{1}{3}}\big].\end{aligned}$$

Now, let $h(t) = \langle t\rangle^{\frac{1}{3}} = (1+t^2)^{\frac{1}{6}}$. We have that

$$h'(t) = \frac{1}{3}t(1+t^2)^{-\frac{5}{6}}, \qquad h''(t) = \frac{1}{9}(3-2t^2)(1+t^2)^{-\frac{11}{6}}, \tag{3.9}$$

so $h', h'' \in L_2(\mathbb{R})$. Hence, by Theorem 2.69, it suffices to check that

$$\big[\langle\mathcal{D}\rangle^{-\frac{k+1}{3}}(\mathbb{I}\otimes M_{f^{\frac{1}{2}}})\langle\mathcal{D}\rangle^{\frac{k}{3}-d}, \mathcal{D}\big] \in \mathcal{L}_1,$$

for each $k = 0,\dots,3d-1$ (that is, the above commutator has bounded extension belonging to $\mathcal{L}_1$). Appealing to Corollary 2.9 above, we obtain the expression

$$\begin{aligned}\big[\langle\mathcal{D}\rangle^{-\frac{k+1}{3}}(\mathbb{I}\otimes M_{f^{\frac{1}{2}}})\langle\mathcal{D}\rangle^{\frac{k}{3}-d}, \mathcal{D}\big] &= \langle\mathcal{D}\rangle^{-\frac{k+1}{3}}[\mathbb{I}\otimes M_{f^{\frac{1}{2}}}, \mathcal{D}]\langle\mathcal{D}\rangle^{\frac{k}{3}-d}\\ &\overset{(2.6)}{=} -\sum_{j=1}^{d}\langle\mathcal{D}\rangle^{-\frac{k+1}{3}}(\gamma_j\otimes M_{\partial_j(f^{\frac{1}{2}})})\langle\mathcal{D}\rangle^{\frac{k}{3}-d}\end{aligned}$$

on the dense domain $\mathbb{C}^{N_d}\otimes W_2^1(\mathbb{R}^d)$. Since the expression on the right-hand side defines a bounded operator on $\mathbb{C}^{N_d}\otimes L_2(\mathbb{R}^d)$, the operator on the left-hand side may be extended to a bounded operator. Furthermore, by Lemma 3.12, we have for every $j = 1,\dots,d$ that $M_{\partial_j(f^{\frac{1}{2}})}\langle\nabla\rangle^{-d-\frac{1}{3}}$ is trace-class. Therefore, by Theorem 2.20, we have

$$\begin{aligned}\big\|\langle\mathcal{D}\rangle^{-\frac{k+1}{3}}(\gamma_j\otimes M_{\partial_j(f^{\frac{1}{2}})})\langle\mathcal{D}\rangle^{\frac{k}{3}-d}\big\|_1 &= \big\|\langle\nabla\rangle^{-\frac{k+1}{3}}M_{\partial_j(f^{\frac{1}{2}})}\langle\nabla\rangle^{\frac{k}{3}-d}\big\|_1\\ &\overset{(2.11)}{\leq} \big\|M_{\partial_j(f^{\frac{1}{2}})}\langle\nabla\rangle^{-d-\frac{1}{3}}\big\|_1 < \infty.\end{aligned}$$

(ii). Suppose $j,k=1,\dots,d$. Observe that

$$\Big[(\mathbb{I}\otimes M_f)^{\frac12},\big(\mathbb{I}\otimes\partial_j\partial_k(-\Delta)^{-1}\big)\langle\mathcal{D}\rangle^{-d}\Big]$$
$$=\mathbb{I}\otimes\big[M_{f^{\frac12}},\partial_j\partial_k(-\Delta)^{-1}\big]\langle\nabla\rangle^{-d}+\big(\mathbb{I}\otimes\partial_j\partial_k(-\Delta)^{-1}\big)\big[\mathbb{I}\otimes M_{f^{\frac12}},\langle\mathcal{D}\rangle^{-d}\big].$$

Hence, by (i), it suffices to show that

$$\big[M_{f^{\frac12}},\partial_j\partial_k(-\Delta)^{-1}\big]\langle\nabla\rangle^{-d}\in\mathcal{L}_1.$$

By Remark 3.10, the operator

$$\partial_j M_{f^{\frac12}}:W_2^1(\mathbb{R}^d)\to L_2(\mathbb{R}^d)$$

is well-defined. Hence, we may write that

$$\big[M_{f^{\frac12}},\partial_j\partial_k(-\Delta)^{-1}\big]\langle\nabla\rangle^{-d}=[M_{f^{\frac12}},\partial_j]\partial_k(-\Delta)^{-1}\langle\nabla\rangle^{-d}+\partial_j\big[M_{f^{\frac12}},(-\Delta)^{-1}\big]\partial_k\langle\nabla\rangle^{-d}$$
$$+\partial_j(-\Delta)^{-1}[M_{f^{\frac12}},\partial_k]\langle\nabla\rangle^{-d}. \tag{3.10}$$

Since $[M_{f^{\frac12}},\partial_j]=M_{\partial_j(f^{\frac12})}\in\mathcal{B}(\mathcal{H})$ by Lemma 2.8, and since $\partial_k(-\Delta)^{-1}$ commutes with $\langle\nabla\rangle^{-d}$, we observe that

$$[M_{f^{\frac12}},\partial_j]\partial_k(-\Delta)^{-1}\langle\nabla\rangle^{-d}=M_{\partial_j(f^{\frac12})}\langle\nabla\rangle^{-d-1}\cdot\langle\nabla\rangle\partial_k(-\Delta)^{-1}.$$

However, by Lemma 3.12, we have that $M_{\partial_j(f^{\frac12})}\langle\nabla\rangle^{-d-1}$ is trace-class. Hence, the first term on the right-hand side of (3.10) belongs to trace-class. Similarly, the third term of (3.10) is given by

$$\partial_j(-\Delta)^{-1}[M_{f^{\frac12}},\partial_k]\langle\nabla\rangle^{-d}=\partial_j\langle\nabla\rangle(-\Delta)^{-1}\cdot\langle\nabla\rangle^{-1}M_{\partial_k(f^{\frac12})}\langle\nabla\rangle^{-d},$$

which also belongs to trace-class due to Theorem 2.20.

It remains to show that the second term on the right-hand side of (3.10) is trace-class. By Lemma 2.2 (i) and the definition of the Laplacian, we have that

$$\partial_j\big[M_{f^{\frac12}},(-\Delta)^{-1}\big]\partial_k\langle\nabla\rangle^{-d}=-\partial_j(-\Delta)^{-1}\Big(\sum_{\ell=1}^d[M_{f^{\frac12}},\partial_\ell^2]\Big)\partial_k(-\Delta)^{-1}\langle\nabla\rangle^{-d}$$
$$=-\sum_{\ell=1}^d\Big(\partial_j\langle\nabla\rangle(-\Delta)^{-1}\big(\langle\nabla\rangle^{-1}M_{\partial_\ell(f^{\frac12})}\langle\nabla\rangle^{-d}\big)\partial_\ell\partial_k(-\Delta)^{-1}$$
$$+\partial_j\partial_\ell(\Delta)^{-1}\big(M_{\partial_\ell(f^{\frac12})}\langle\nabla\rangle^{-d-1}\big)\langle\nabla\rangle\partial_k(-\Delta)^{-1}\Big),$$

and, by appealing to Lemma 3.12 and Theorem 2.20 as above, we observe that each term in the summation on the right-hand side also belongs to trace-class. $\square$

Finally, to explicitly calculate the Dixmier trace of $(\mathbb{I}\otimes M_f)\langle\mathcal{D}\rangle^{-d}$ using Theorem 3.7, we need to establish existence of the relevant limit.

Proposition 3.14. *If $0 \le f \in \mathcal{S}(\mathbb{R}^d)$, then the limit*

$$\lim_{\varepsilon\downarrow 0} \varepsilon \operatorname{Tr}\big((\mathbb{I}\otimes M_f)^{1+\varepsilon}\langle\mathcal{D}\rangle^{-d(1+\varepsilon)}\big) \text{ exists.}$$

In particular, $(\mathbb{I}\otimes M_f)\langle\mathcal{D}\rangle^{-d}$ is a Dixmier measurable operator on $\mathbb{C}^{N_d}\otimes L_2(\mathbb{R}^d)$ and, for any extended limit ω,

$$\operatorname{Tr}_\omega\big((\mathbb{I}\otimes M_f)\langle\mathcal{D}\rangle^{-d}\big) = \frac{2^{\lfloor \frac{d}{2}\rfloor}\operatorname{Vol}(\mathbb{S}^{d-1})}{d(2\pi)^d}\int_{\mathbb{R}^d} f(\mathbf{x})\,\mathrm{d}\mathbf{x},$$

where $\operatorname{Vol}(\mathbb{S}^{d-1})$ denotes the volume of the unit hypersphere $\mathbb{S}^{d-1}$.

Proof. We wish to apply Theorem 3.7 for $A = \mathbb{I}\otimes M_f$ and $B = \langle\mathcal{D}\rangle^{-d}$.

Step 1: We verify that, for every $0<\varepsilon<1$, the operator $B^{1+\varepsilon}A^{1+\varepsilon}$ is trace class. Since $\langle\mathcal{D}\rangle^{-d(1+\varepsilon)} = \mathbb{I}\otimes\langle\nabla\rangle^{-d(1+\varepsilon)}$, we observe that

$$B^{1+\varepsilon}A^{1+\varepsilon} = \mathbb{I}\otimes\big(\langle\nabla\rangle^{-d(1+\varepsilon)}M_f^{1+\varepsilon}\big). \tag{3.11}$$

However, the classical trace on $\mathcal{L}_1\big(\mathbb{C}^{N_d}\otimes L_2(\mathbb{R}^d)\big) \simeq M_{N_d}(\mathbb{C})\otimes\mathcal{L}_1\big(L_2(\mathbb{R}^d)\big)$ is given by $\operatorname{tr}\otimes\operatorname{Tr}$, where tr is the matrix trace on $M_{N_d}(\mathbb{C})$ and Tr is the classical trace on $\mathcal{L}_1\big(L_2(\mathbb{R}^d)\big)$. That is, if either of the relevant norms exist, then we have the identity

$$\|B^{1+\varepsilon}A^{1+\varepsilon}\|_1 = N_d\big\|\langle\nabla\rangle^{-d(1+\varepsilon)}M_f^{1+\varepsilon}\big\|_1.$$

Since $0<\frac{1}{1+\varepsilon}<1$, it follows from (2.16) that

$$\|f^{1+\varepsilon}\|_{\ell_1(L_2)} \overset{(2.16)}{=} \|f\|^{1+\varepsilon}_{\ell_{1+\varepsilon}(L_{2(1+\varepsilon)})} < \infty,$$

and therefore that $f^{1+\varepsilon}\in\ell_1(L_2)(\mathbb{R}^d)$, for every $0<\varepsilon<1$. Hence, by Remark 2.49 and Theorem 2.50, the operator $M_f^{1+\varepsilon}\langle\nabla\rangle^{-d(1+\varepsilon)}$ is trace class for all $0<\varepsilon<1$, and so is its adjoint $\langle\nabla\rangle^{-d(1+\varepsilon)}M_f^{1+\varepsilon}$ by symmetry.

Step 2: We now calculate $\operatorname{Tr}\big(\langle\nabla\rangle^{-d(1+\varepsilon)}M_f^{1+\varepsilon}\big)$ for $\varepsilon>0$. We do so by considering $\langle\nabla\rangle^{-d(1+\varepsilon)}M_f^{1+\varepsilon}$ as an integral operator. Observe that

$$\big(\langle\nabla\rangle^{-d(1+\varepsilon)}\phi\big)(\mathbf{x}) = \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d}\mathcal{F}^{-1}\big[\langle\cdot\rangle^{-d(1+\varepsilon)}\big](\mathbf{x}-\mathbf{y})\phi(\mathbf{y})\,\mathrm{d}\mathbf{y},\quad \phi\in L_2(\mathbb{R}^d),\ \mathbf{x}\in\mathbb{R}^d.$$

Hence, $\langle\nabla\rangle^{-d(1+\varepsilon)}M_f^{1+\varepsilon}$ has an integral kernel given by the expression

$$K(\mathbf{x},\mathbf{y}) := \frac{1}{(2\pi)^{\frac{d}{2}}}f(\mathbf{y})^{1+\varepsilon}\cdot\mathcal{F}^{-1}\big[\langle\cdot\rangle^{-d(1+\varepsilon)}\big](\mathbf{x}-\mathbf{y}),\quad \mathbf{x},\mathbf{y}\in\mathbb{R}^d,$$

which is continuous [70, Theorem IX.7] and, by the Fubini–Tonelli theorem, belongs to $L_2(\mathbb{R}^d \times \mathbb{R}^d)$, so we may appeal to Proposition 2.32 to get that

$$\begin{aligned}
\operatorname{Tr}(B^{1+\varepsilon}A^{1+\varepsilon}) &\overset{(3.11)}{=} N_d \operatorname{Tr}\big(\langle\nabla\rangle^{-d(1+\varepsilon)} M_f^{1+\varepsilon}\big) = N_d \int_{\mathbb{R}^d} K(\mathbf{x},\mathbf{x})\,\mathrm{d}\mathbf{x} \\
&= \frac{N_d}{(2\pi)^{\frac{d}{2}}} \int_{\mathbb{R}^d} f(\mathbf{x})^{1+\varepsilon} \cdot \mathcal{F}^{-1}\big[\langle\cdot\rangle^{-d(1+\varepsilon)}\big](\mathbf{0})\,\mathrm{d}\mathbf{x} \\
&= \frac{N_d}{(2\pi)^d}\Big(\int_{\mathbb{R}^d} \langle\mathbf{s}\rangle^{-d(1+\varepsilon)}\,\mathrm{d}\mathbf{s}\Big)\Big(\int_{\mathbb{R}^d} f(\mathbf{x})^{1+\varepsilon}\,\mathrm{d}\mathbf{x}\Big) \\
&= \frac{N_d \operatorname{Vol}(\mathbb{S}^{d-1})\Gamma\big(\frac{d}{2}\big)\Gamma\big(\frac{d\varepsilon}{2}\big)}{2(2\pi)^d\Gamma\big(\frac{d(1+\varepsilon)}{2}\big)} \int_{\mathbb{R}^d} f(\mathbf{x})^{1+\varepsilon}\,\mathrm{d}\mathbf{x},
\end{aligned} \tag{3.12}$$

where in the last line we appealed to [1, §6.2]. Since $f^{1+\varepsilon} \to f$ pointwise as $\varepsilon \downarrow 0$, the dominated convergence theorem yields

$$\lim_{\varepsilon\downarrow 0} \int_{\mathbb{R}^d} f(\mathbf{x})^{1+\varepsilon}\,\mathrm{d}\mathbf{x} = \int_{\mathbb{R}^d} f(\mathbf{x})\,\mathrm{d}\mathbf{x}. \tag{3.13}$$

Since

$$\lim_{\varepsilon\downarrow 0} \varepsilon\Gamma\Big(\frac{d\varepsilon}{2}\Big) = \frac{2}{d}\lim_{\varepsilon\downarrow 0}\Gamma\Big(\frac{d\varepsilon}{2}+1\Big) = \frac{2}{d}, \tag{3.14}$$

the limit in Proposition 3.7 exists and is given by the expression

$$\begin{aligned}
\lim_{\varepsilon\downarrow 0} \varepsilon \operatorname{Tr}\big(\langle\mathcal{D}\rangle^{-d(1+\varepsilon)}(\mathbb{I}\otimes M_f)^{1+\varepsilon}\big) &\overset{(3.12)}{=} \frac{N_d \operatorname{Vol}(\mathbb{S}^{d-1})\Gamma\big(\frac{d}{2}\big)}{2(2\pi)^d} \lim_{\varepsilon\downarrow 0}\Big(\frac{\varepsilon\,\Gamma\big(\frac{d\varepsilon}{2}\big)}{\Gamma\big(\frac{d(1+\varepsilon)}{2}\big)}\int_{\mathbb{R}^d} f(\mathbf{x})^{1+\varepsilon}\,\mathrm{d}\mathbf{x}\Big) \\
&= \frac{N_d \operatorname{Vol}(\mathbb{S}^{d-1})}{d(2\pi)^d}\int_{\mathbb{R}^d} f(\mathbf{x})\,\mathrm{d}\mathbf{x}.
\end{aligned}$$

Finally, appealing to Lemma 3.13 (i), the conditions of Proposition 3.7 are satisfied. Therefore, $(\mathbb{I}\otimes M_f)\langle\mathcal{D}\rangle^{-d}$ is Dixmier measurable, and we have that the Dixmier trace $\operatorname{Tr}_\omega\big((\mathbb{I}\otimes M_f)\langle\mathcal{D}\rangle^{-d}\big)$ agrees with the above, for any extended limit ω. □

By a similar argument, we may also obtain the following special case of Connes' trace theorem, which we require as a technical lemma for Section 4.1.4 below.

Lemma 3.15. *Let $d \geq 2$. If $0 \leq f \in \mathcal{S}(\mathbb{R}^d)$, then the limit*

$$\lim_{\varepsilon\downarrow 0} \varepsilon \operatorname{Tr}\Big((\mathbb{I}\otimes M_f)^{1+\varepsilon}\big(\mathbb{I}\otimes\partial_j\partial_k(-\Delta)^{-1}\big)^{1+\varepsilon}\langle\mathcal{D}\rangle^{-d(1+\varepsilon)}\Big) \text{ exists,}$$

for all $j,k = 1,\dots,d$. In particular, $(\mathbb{I}\otimes M_f)\big(\mathbb{I}\otimes\partial_j\partial_k(-\Delta)^{-1}\big)\langle\mathcal{D}\rangle^{-d}$ is a Dixmier measurable operator on $\mathbb{C}^{N_d}\otimes L_2(\mathbb{R}^d)$ and there exists a constant $C_d > 0$ depending only on d such that, for any extended limit ω,

$$\operatorname{Tr}_\omega\Big((\mathbb{I}\otimes M_f)\big(\mathbb{I}\otimes\partial_j\partial_k(-\Delta)^{-1}\big)\langle\mathcal{D}\rangle^{-d}\Big) = \delta_{j,k}C_d\int_{\mathbb{R}^d} f(\mathbf{x})\,\mathrm{d}\mathbf{x},$$

where $\delta_{j,k}$ denotes the Kronecker delta for $j,k = 1,\dots,d$.

Proof. We wish to apply Theorem 3.7 for the bounded operators

$$A = \mathbb{I} \otimes M_f \quad \text{and} \quad B_\pm = \big(\mathbb{I} \otimes h^\pm_{j,k}(\nabla)\big)\langle \mathcal{D}\rangle^{-d},$$

where $h^\pm_{j,k} \in (L_{1,\infty} \cap L_\infty)(\mathbb{R}^d)$ are the nonnegative-valued functions defined by the expressions

$$h^+_{j,k}(\mathbf{t}) := \frac{|t_j t_k|}{|\mathbf{t}|^2\langle \mathbf{t}\rangle^d}, \quad h^-_{j,k}(\mathbf{t}) := \frac{|t_j t_k| - t_j t_k}{|\mathbf{t}|^2\langle \mathbf{t}\rangle^d}, \quad \mathbf{t} \in \mathbb{R}^d.$$

Since $\mathbb{I} \otimes h^\pm_{j,k}(\nabla)$ are bounded operators via the Borel functional calculus, and since $(\mathbb{I} \otimes M_f)^{1+\varepsilon}\langle \mathcal{D}\rangle^{-d(1+\varepsilon)} \in \mathcal{L}_1$ by Lemma 3.12, we have that $B_\pm^{1+\varepsilon}A^{1+\varepsilon}$ is trace-class, for every $0 < \varepsilon < 1$.

We now calculate the classical trace of $B_\pm^{1+\varepsilon}A^{1+\varepsilon}$ for $\varepsilon > 0$, which may be done by considering them as integral operators. Observe that $(h^\pm_{j,k})^{1+\varepsilon} \in L_1(\mathbb{R}^d)$, for all $\varepsilon > 0$, so $\mathcal{F}^{-1}\big[(h^\pm_{j,k})^{1+\varepsilon}\big]$ is continuous [70, Theorem IX.7]. Moreover, we have that

$$\begin{aligned}\big((h^\pm_{j,k})^{1+\varepsilon}(\nabla)\phi\big)(\mathbf{x}) &= (\mathcal{F}^{-1}M^{1+\varepsilon}_{h^\pm_{j,k}}\mathcal{F}\phi)(\mathbf{x})\\ &= \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d} \mathcal{F}^{-1}\big[(h^\pm_{j,k})^{1+\varepsilon}\big](\mathbf{x}-\mathbf{t})\phi(\mathbf{t})\,\mathrm{d}\mathbf{t}, \quad \phi \in L_2(\mathbb{R}^d),\ \mathbf{x} \in \mathbb{R}^d.\end{aligned}$$

Hence, the integral kernel of $(h^\pm_{j,k})^{1+\varepsilon}(\nabla)M_f(1+\varepsilon)$ is given by the expression

$$K(\mathbf{x},\mathbf{t}) := \frac{1}{(2\pi)^{\frac{d}{2}}} f^{1+\varepsilon}(\mathbf{t}) \cdot \mathcal{F}^{-1}\big[(h^\pm_{j,k})^{1+\varepsilon}\big](\mathbf{x}-\mathbf{t}), \quad \text{for } \mathbf{x},\mathbf{t} \in \mathbb{R}^d,$$

which is continuous and, by the Fubini–Tonelli theorem, belongs to $L_2(\mathbb{R}^d \times \mathbb{R}^d)$. Hence, we may appeal to Proposition 2.32 to obtain the expression

$$\begin{aligned}\mathrm{Tr}(B_\pm^{1+\varepsilon}A^{1+\varepsilon}) &= N_d\,\mathrm{Tr}\left(M_f^{1+\varepsilon}(h^\pm_{j,k})^{1+\varepsilon}(\nabla)\right) = N_d\int_{\mathbb{R}^d} K(\mathbf{x},\mathbf{x})\,\mathrm{d}\mathbf{x}\\ &= \frac{N_d}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d} f^{1+\varepsilon}(\mathbf{x})\cdot\mathcal{F}^{-1}\big[(h^\pm_{j,k})^{1+\varepsilon}\big](\mathbf{0})\,\mathrm{d}\mathbf{x}\\ &= \frac{N_d}{(2\pi)^d}\int_{\mathbb{R}^d}(h^\pm_{j,k})^{1+\varepsilon}(\mathbf{t})\,\mathrm{d}\mathbf{t}\cdot\int_{\mathbb{R}^d} f^{1+\varepsilon}(\mathbf{x})\,\mathrm{d}\mathbf{x}.\end{aligned}$$

First, we calculate $\lim_{\varepsilon\downarrow 0}\varepsilon\,\mathrm{Tr}(B_+^{1+\varepsilon}A^{1+\varepsilon})$. We may pass to polar coordinates and appeal to [1, §6.2] to obtain the integral

$$\begin{aligned}\int_{\mathbb{R}^d}(h^+_{j,k})^{1+\varepsilon}(\mathbf{t})\,\mathrm{d}\mathbf{t} &= \left(\int_0^\infty \frac{r^{d-1}}{(1+r^2)^{\frac{d(1+\varepsilon)}{2}}}\,\mathrm{d}r\right)\left(\int_\Omega u_{\delta_{j,k}}(\mathbf{s},\varepsilon)\,\mathrm{d}\mathbf{s}\right)\\ &= \frac{\Gamma(\frac{d}{2})\Gamma(\frac{d\varepsilon}{2})}{2\Gamma(\frac{d(1+\varepsilon)}{2})}\int_\Omega u_{\delta_{j,k}}(\mathbf{s},\varepsilon)\,\mathrm{d}\mathbf{s},\end{aligned} \tag{3.15}$$

where Γ is the usual Gamma function, Ω denotes the compact set $[0,\pi]^{d-2}\times[0,2\pi] \subset \mathbb{R}^{d-1}$, and u_0, u_1 are the continuous, uniformly bounded functions on $\Omega \times [0,\infty)$ given by the expressions

$$u_0(\mathbf{s},\varepsilon) := \big|\cos(s_1)\sin(s_1)\cos(s_2)\big|^{1+\varepsilon}\prod_{\ell=1}^{d-2}\sin^{d-\ell-1}(s_j),$$

$$u_1(\mathbf{s},\varepsilon) := \big|\cos(s_1)^2\big|^{1+\varepsilon}\prod_{\ell=1}^{d-2}\sin^{d-\ell-1}(s_j), \quad \text{for } \mathbf{s}=(s_1,\dots,s_{d-1})\in\Omega,\ \varepsilon\geq 0.$$

By the dominated convergence theorem, we observe that

$$\lim_{\varepsilon\downarrow 0}\int_\Omega u_m(\mathbf{t},\varepsilon)\,\mathrm{d}\mathbf{t} = \int_\Omega u_m(\mathbf{t},0)\,\mathrm{d}\mathbf{t} =: a_m < \infty, \quad \text{for each } m=0,1.$$

Therefore, by (3.13) and (3.14), we obtain the limit

$$\lim_{\varepsilon\downarrow 0}\varepsilon\,\mathrm{Tr}(B_+^{1+\varepsilon}A^{1+\varepsilon}) = \frac{a_{\delta_{j,k}}N_d}{d(2\pi)^d}\cdot\int_{\mathbb{R}^d}f(\mathbf{x})\,\mathrm{d}\mathbf{x} = a'_{\delta_{j,k}}\int_{\mathbb{R}^d}f(\mathbf{x})\,\mathrm{d}\mathbf{x}, \tag{3.16}$$

where $a'_m := \frac{a_m N_d}{d(2\pi)^d} > 0$, for each $m=0,1$.

Next, we calculate $\lim_{\varepsilon\downarrow 0}\varepsilon\,\mathrm{Tr}(B_-^{1+\varepsilon}A^{1+\varepsilon})$. By a similar argument to (3.15), one has the integral

$$\int_{\mathbb{R}^d}(h_{j,k}^-)^{1+\varepsilon}(\mathbf{t})\,\mathrm{d}\mathbf{t} = \frac{\Gamma(\frac{d}{2})\Gamma(\frac{d\varepsilon}{2})}{2\Gamma(\frac{d(1+\varepsilon)}{2})}\int_\Omega v_{\delta_{j,k}}(\mathbf{t},\varepsilon)\,\mathrm{d}\mathbf{t},$$

where v_0, v_1 are the continuous, uniformly bounded functions on $\Omega\times[0,\infty)$ given by the expressions

$$v_0(\mathbf{s},\varepsilon) := \Big(\big|\cos(s_1)\sin(s_1)\cos(s_2)\big| - \cos(s_1)\sin(s_1)\cos(s_2)\Big)^{1+\varepsilon}\prod_{\ell=1}^{d-2}\sin^{d-\ell-1}(s_\ell),$$

$$v_1(\mathbf{s},\varepsilon) := \Big(\big|\cos(s_1)^2\big| - \cos(s_1)^2\Big)^{1+\varepsilon}\prod_{\ell=1}^{d-2}\sin^{d-\ell-1}(s_\ell), \quad \text{for } \mathbf{s}\in\Omega,\ \varepsilon\geq 0.$$

Note that the values of v_0, v_1 at $\varepsilon=0$ are given by

$$v_0(\mathbf{s},0) = u_0(\mathbf{s},0) - \cos(s_1)\sin(s_1)\cos(s_2)\prod_{\ell=1}^{d-2}\sin^{d-\ell-1}(s_\ell),$$

$$v_1(\mathbf{s},0) = u_1(\mathbf{s},0) - \cos^2(s_1)\prod_{\ell=1}^{d-2}\sin^{d-\ell-1}(s_\ell), \quad \text{for all } \mathbf{s}\in\Omega.$$

Hence, the dominated convergence theorem implies that

$$\lim_{\varepsilon\downarrow 0}\int_\Omega v_m(\mathbf{t},\varepsilon)\,\mathrm{d}\mathbf{t} = \int_\Omega v_m(\mathbf{t},0)\,\mathrm{d}\mathbf{t} = \begin{cases} a_0 - C''_d, & \text{if } m=0,\\ a_1 - C'_d, & \text{if } m=1,\end{cases}$$

$$= a_m - mC'_d, \quad \text{for each } m=0,1,$$

where

$$C'_d := \int_\Omega \cos^2(s_1)\prod_{\ell=1}^{d-2}\sin^{d-\ell-1}(s_\ell)\,\mathrm{d}\mathbf{s} > 0,$$

and since

$$C_d'' := \int_\Omega \cos(s_1)\sin(s_1)\cos(s_2)\prod_{\ell=1}^{d-2}\sin^{d-\ell-1}(s_\ell)\,\mathrm{d}\mathbf{s} = 0.$$

Hence, by a similar argument to (3.16) above, we have that

$$\lim_{\varepsilon\downarrow 0}\varepsilon\,\mathrm{Tr}(B_-^{1+\varepsilon}A^{1+\varepsilon}) = (a'_{\delta_{j,k}} - \delta_{j,k}C_d)\int_{\mathbb{R}^d} f(\mathbf{x})\,\mathrm{d}\mathbf{x},$$

where $C_d := N_d(2\pi)^d C_d' > 0$ depends only on d.

Appealing to Lemma 3.13 (ii), we observe that the conditions of Proposition 3.7 are satisfied. Therefore, $(\mathbb{I}\otimes M_f)\big(\mathbb{I}\otimes(h_{j,k}^{\pm})(\nabla)\big)\langle\mathcal{D}\rangle^{-d}$ is Dixmier measurable and

$$\begin{aligned}\mathrm{Tr}_\omega\left((\mathbb{I}\otimes M_f)\big(\mathbb{I}\otimes\partial_j\partial_k(-\Delta)^{-1}\big)\langle\mathcal{D}\rangle^{-d}\right) &= \mathrm{Tr}_\omega(AB_+) - \mathrm{Tr}_\omega(AB_-)\\ &= \lim_{\varepsilon\downarrow 0}\varepsilon\,\mathrm{Tr}(B_+^{1+\varepsilon}A^{1+\varepsilon}) - \lim_{\varepsilon\downarrow 0}\varepsilon\,\mathrm{Tr}(B_-^{1+\varepsilon}A^{1+\varepsilon}) = \delta_{j,k}C_d\int_{\mathbb{R}^d} f(\mathbf{x})\,\mathrm{d}\mathbf{x},\end{aligned}$$

for any extended limit ω. □

Theorem 3.16. *If $f\in W_1^d(\mathbb{R}^d)$, then $(\mathbb{I}\otimes M_f)\langle\mathcal{D}\rangle^{-d}$ is a Dixmier measurable operator on $\mathbb{C}^{N_d}\otimes L_2(\mathbb{R}^d)$ and, for any extended limit ω,*

$$\mathrm{Tr}_\omega\left((\mathbb{I}\otimes M_f)\langle\mathcal{D}\rangle^{-d}\right) = \frac{2^{\lfloor\frac{d}{2}\rfloor}\,\mathrm{Vol}(\mathbb{S}^{d-1})}{d(2\pi)^d}\int_{\mathbb{R}^d} f(\mathbf{x})\,\mathrm{d}\mathbf{x},$$

where $\mathrm{Vol}(\mathbb{S}^{d-1})$ denotes the volume of the unit hypersphere $\mathbb{S}^{d-1}$.

Proof. Without loss of generality, assume f is nonnegative. Since $\mathcal{S}(\mathbb{R}^d)$ is dense in the Sobolev space $W_1^d(\mathbb{R}^d)$, one may construct a sequence $\{f_n\}_{n\in\mathbb{N}}$ of nonnegative Schwartz functions on $\mathbb{R}^d$ such that $f_n\to f$ in $W_1^d(\mathbb{R}^d)$. Then, by Proposition 2.56 (with $p=1$, $\delta=d$), we have

$$\left\|M_f\langle\nabla\rangle^{-d} - M_{f_n}\langle\nabla\rangle^{-d}\right\|_{1,\infty} \le \mathrm{const}\cdot\|f-f_n\|_{W_1^d}\to 0.$$

Hence, the sequence of operators $\left\{M_{f_n}\langle\nabla\rangle^{-d}\right\}_{n\in\mathbb{N}}$ converges to $M_f\langle\nabla\rangle^{-d}$ in $\mathcal{L}_{1,\infty}$. Therefore, since Tr_ω is continuous on $\mathcal{L}_{1,\infty}$,

$$\begin{aligned}\mathrm{Tr}_\omega\left((\mathbb{I}\otimes M_f)\langle\mathcal{D}\rangle^{-d}\right) = N_d\lim_{n\to\infty}\mathrm{Tr}_\omega\left(M_{f_n}\langle\nabla\rangle^{-d}\right) &= \frac{N_d\,\mathrm{Vol}(\mathbb{S}^{d-1})}{d(2\pi)^d}\lim_{n\to\infty}\int_{\mathbb{R}^d} f_n(\mathbf{x})\,\mathrm{d}\mathbf{x}\\ &= \frac{N_d\,\mathrm{Vol}(\mathbb{S}^{d-1})}{d(2\pi)^d}\int_{\mathbb{R}^d} f(\mathbf{x})\,\mathrm{d}\mathbf{x},\end{aligned}$$

where in the second equality we appealed to Proposition 3.14. □

3.4 Connes integration formula for the Moyal plane

In this section, we obtain an analogue of Theorem 3.16 for the noncommutative plane. The reader is advised that any unexplained notations are properly defined in Section 3.4.1 below.

We consider the Fréchet $*$-algebra $\mathcal{S}(\mathbb{R}^2_\Theta)$, which is a representation of the algebra of Schwartz functions $\big(\mathcal{S}(\mathbb{R}^2), \diamond_\Theta\big)$ in the type I_∞ von Neumann algebra $L_\infty(\mathbb{R}^2_\Theta)$. Here, the binary operation $\diamond_\Theta$ on $\mathcal{S}(\mathbb{R}^2)$ is a noncommutative analogue of the convolution product parametrised by a real-valued nonzero anti-symmetric matrix $\Theta \in M_2(\mathbb{R})$. This space has been studied previously in [41], which established an isomorphism between $\mathcal{S}(\mathbb{R}^2_\Theta)$ and the algebra $\mathbf{S}$ of "infinite matrices with rapidly decreasing entries".

Using this isomorphism, we deduce that $\mathcal{S}(\mathbb{R}^2_\Theta)$ has a nontrivial positive cone and that, if $f \in \mathcal{S}(\mathbb{R}^2)$ is represented in $\mathcal{S}(\mathbb{R}^2_\Theta)$ by a positive operator, then there exists some $g \in \mathcal{S}(\mathbb{R}^2)$ such that $g \diamond_\Theta g = f$ (see Corollary 3.42 below). The invariance of the space of Schwartz elements under the square root operation is a feature of the noncommutivity of $\diamond_\Theta$. We shall observe that the estimate

$$\big[\mathrm{Op}_\Theta(f)^{\frac{1}{2}}, (1-\Delta_\Theta)^{-1}\big] \in \mathcal{L}_1, \quad 0 \le \mathrm{Op}_\Theta(f) \in \mathcal{S}(\mathbb{R}^2_\Theta)$$

(where $\mathrm{Op}_\Theta(f)$ and Δ_Θ are defined in Section 3.4.1 below) follows from the fact that $\mathcal{S}(\mathbb{R}^2_\Theta)$ is naturally embedded in the noncommutative analogue of Sobolev space $W^2_1(\mathbb{R}^2_\Theta)$ defined in [53] (see, e.g., [86, Lemma 3.3]). Then Theorem 1.1 can be used to show (see Proposition 3.45 below) that

$$\mathrm{Tr}_\omega\big(\mathrm{Op}_\Theta(f)(1-\Delta_\Theta)^{-1}\big) = \pi f(\mathbf{0}).$$

This trace formula was previously shown in [86] for $X(1-\Delta_\Theta)^{-1}$, for any $X \in W^2_1(\mathbb{R}^2_\Theta)$ [86, Theorem 1.1], but the argument and approach here are new. By a density argument, we recover the result in [86] in Corollary 3.46 below.

The definitions in this section are derived from [41, 42, 35, 53].

3.4.1 Definition of the Moyal plane

Noncommutative Euclidean space may be defined for arbitrary dimension $d \in \mathbb{Z}_+$ and arbitrary anti-symmetric $\Theta \in M_d(\mathbb{R})$, and is denoted $L_\infty(\mathbb{R}^d_\Theta)$. However, since [53, Corollary 6.4] gives a von Neumann algebra isomorphism

$$L_\infty(\mathbb{R}^d_\Theta) \simeq \underbrace{L_\infty(\mathbb{R}^2_S)\bar{\otimes}\cdots\bar{\otimes}L_\infty(\mathbb{R}^2_S)}_{\frac{1}{2}\mathrm{rank}(\Theta)\text{ times}} \bar{\otimes} \underbrace{L_\infty(\mathbb{R})\bar{\otimes}\cdots\bar{\otimes}L_\infty(\mathbb{R})}_{\mathrm{null}(\Theta)\text{ times}},$$

where $S = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, we shall only consider the 2-dimensional noncommutative Euclidean space, also known as Moyal plane.

Definition 3.17. Let $\theta \in \mathbb{R}$, and let $\Theta = \begin{pmatrix} 0 & \theta \\ -\theta & 0 \end{pmatrix}$. Define a bilinear form on $\mathbb{R}^2$ by

$$\langle \mathbf{x}, \mathbf{y} \rangle_\Theta := \mathbf{x} \cdot \Theta \mathbf{y} = \theta(x_1 y_2 - x_2 y_1), \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^2.$$

Remark 3.18. Observe that the skew-symmetry of Θ implies the skew-symmetry of $\langle \cdot, \cdot \rangle_\Theta$; that is,

$$\langle \mathbf{x}, \mathbf{y} \rangle_\Theta = -\langle \mathbf{y}, \mathbf{x} \rangle_\Theta, \text{ for all } \mathbf{x}, \mathbf{y} \in \mathbb{R}^2. \tag{3.17}$$

For each $\mathbf{t} \in \mathbb{R}^2$, define an operator $U_{\mathbf{t}}^\Theta$ on $L_2(\mathbb{R}^2)$ by

$$(U_{\mathbf{t}}^\Theta f)(\mathbf{x}) := e^{-i\langle \mathbf{t}, \mathbf{x} \rangle_\Theta} f(\mathbf{x} - \mathbf{t}), \quad f \in L_2(\mathbb{R}^2),\, \mathbf{x} \in \mathbb{R}^2.$$

Remark 3.19. For every $\mathbf{s}, \mathbf{t} \in \mathbb{R}^2$, we have that

$$U_{\mathbf{t}}^\Theta U_{\mathbf{s}}^\Theta = e^{-i\langle \mathbf{t}, \mathbf{s} \rangle_\Theta} U_{\mathbf{t}+\mathbf{s}}^\Theta, \quad \mathbf{s}, \mathbf{t} \in \mathbb{R}^2. \tag{3.18}$$

In particular, $(U_{\mathbf{t}}^\Theta)^{-1} = U_{-\mathbf{t}}^\Theta$, for all $\mathbf{t} \in \mathbb{R}^2$.

Proof. Observe that, for all $f \in L_2(\mathbb{R}^2)$ and all $\mathbf{x} \in \mathbb{R}^2$, we have

$$\begin{aligned}(U_{\mathbf{t}}^\Theta U_{\mathbf{s}}^\Theta f)(\mathbf{x}) &= e^{-i\langle \mathbf{t}, \mathbf{x} \rangle_\Theta} (U_{\mathbf{s}}^\Theta f)(\mathbf{x} - \mathbf{t}) = e^{-i\langle \mathbf{t}, \mathbf{x} \rangle_\Theta} e^{-i\langle \mathbf{s}, \mathbf{x} - \mathbf{t} \rangle_\Theta} f(\mathbf{x} - \mathbf{t} - \mathbf{s}) \\ &= e^{i\langle \mathbf{s}, \mathbf{t} \rangle_\Theta} (U_{\mathbf{t}+\mathbf{s}}^\Theta f)(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^2. \end{aligned}$$ □

Remark 3.20. For every $\mathbf{t} \in \mathbb{R}^2$, $U_{\mathbf{t}}^\Theta$ is unitary.

Proof. By the previous remark, it suffices to show that $(U_{\mathbf{t}}^\Theta)^* = U_{-\mathbf{t}}^\Theta$, for any $\mathbf{t} \in \mathbb{R}^2$. Indeed, for all $f, g \in \mathbb{R}^2$, we have that

$$\langle U_{\mathbf{t}}^\Theta f, g \rangle = \int_{\mathbb{R}^2} e^{-i\langle \mathbf{t}, \mathbf{x} \rangle_\Theta} f(\mathbf{x} - \mathbf{t}) \overline{g(\mathbf{x})} \, \mathrm{d}\mathbf{x} = \int_{\mathbb{R}^2} f(\mathbf{x}) \overline{e^{i\langle \mathbf{t}, \mathbf{x}+\mathbf{t} \rangle_\Theta} g(\mathbf{x} + \mathbf{t})} \, \mathrm{d}\mathbf{x} = \langle f, U_{-\mathbf{t}}^\Theta g \rangle.$$ □

Definition 3.21. The von Neumann algebra on $L_2(\mathbb{R}^2)$ generated by the family $\{U_{\mathbf{t}}^\Theta\}_{\mathbf{t} \in \mathbb{R}^2}$ is called the *Moyal plane*, and is denoted by $L_\infty(\mathbb{R}^2_\Theta)$.

Remark 3.22. $L_\infty(\mathbb{R}^2_\Theta)$ is $*$-isomorphic to $\mathcal{B}(L_2(\mathbb{R}^2))$ (see, e.g., [53, Theorem 6.5]). Therefore, it is equipped with a canonical trace τ (for the definition of a trace on a von Neumann algebra and the various definitions of its properties, the reader is referred to [57]). The faithful, normal, semifinite trace τ is the classical trace on $\mathcal{B}(L_2(\mathbb{R}^d))$ composed with the $*$-isomorphism.

In $L_\infty(\mathbb{R}^2_\Theta)$, we may define an algebra of "multiplication operators" corresponding to the Schwartz functions. Unlike the Euclidean case, this algebra is designed to be noncommutative in nature.

Definition 3.23. For a Schwartz function $f \in \mathcal{S}(\mathbb{R}^2)$, define the operator $\mathrm{Op}_\Theta(f) \in L_\infty(\mathbb{R}^2_\Theta)$ by

$$\mathrm{Op}_\Theta(f) \coloneqq \int_{\mathbb{R}^2} f(\mathbf{t}) U^\Theta_{\mathbf{t}} \, \mathrm{d}\mathbf{t}, \tag{3.19}$$

where the integral on the right-hand side may be understood as a Bochner integral. The family of such operators,

$$\mathcal{S}(\mathbb{R}^2_\Theta) \coloneqq \big\{ \mathrm{Op}_\Theta(f) : \, f \in \mathcal{S}(\mathbb{R}^2) \big\},$$

is called *noncommutative Schwartz space.*

Remark 3.24. Observe that, for every $f \in \mathcal{S}(\mathbb{R}^2)$, we have

$$\begin{aligned}\big(\mathrm{Op}_\Theta(f)g\big)(\mathbf{x}) &= \int_{\mathbb{R}^2} f(\mathbf{t}) e^{-i\langle \mathbf{t},\mathbf{x}\rangle_\Theta} g(\mathbf{x}-\mathbf{t}) \, \mathrm{d}\mathbf{t} \\ &= \int_{\mathbb{R}^2} f(\mathbf{x}-\mathbf{t}) e^{i\langle \mathbf{t},\mathbf{x}\rangle_\Theta} g(\mathbf{t}) \, \mathrm{d}\mathbf{t}, \quad g \in L_2(\mathbb{R}^d),\, \mathbf{x} \in \mathbb{R}^2.\end{aligned}$$

Hence, $\mathrm{Op}_\Theta(f)$ is an integral operator whose integral kernel K is given by

$$K(\mathbf{x},\mathbf{t}) \coloneqq f(\mathbf{x}-\mathbf{t}) e^{i\langle \mathbf{t},\mathbf{x}\rangle_\Theta}, \quad \mathbf{x},\mathbf{t} \in \mathbb{R}^2.$$

Remark 3.25. When f and g are Schwartz functions, we have

$$\mathrm{Op}_\Theta(f) + \mathrm{Op}_\Theta(g) = \mathrm{Op}_\Theta(f+g), \quad \mathrm{Op}_\Theta(f) \circ \mathrm{Op}_\Theta(g) = \mathrm{Op}_\Theta(f \diamond_\Theta g),$$

where $\diamond_\Theta$ denotes the "twisted" convolution

$$(f \diamond_\Theta g)(\mathbf{x}) = \int_{\mathbb{R}^2} f(\mathbf{t}) g(\mathbf{x}-\mathbf{t}) e^{-i\langle \mathbf{t},\mathbf{x}\rangle_\Theta} \, \mathrm{d}\mathbf{t}, \quad \mathbf{x} \in \mathbb{R}^2.$$

The Schwartz functions equipped with the associative product $\diamond_\Theta$ forms a Fréchet algebra [41]. Therefore, Op_Θ is a $*$-isomorphism between the algebras $\big(\mathcal{S}(\mathbb{R}^2), \diamond_\Theta\big)$ and $\mathcal{S}(\mathbb{R}^2_\Theta)$.

The operation $\diamond_\Theta$ is a noncommutative analogue of the classical convolution product, and *not* the pointwise product. However, one may consider elements of $\mathcal{S}(\mathbb{R}^2_\Theta)$ as operators from the Fourier dual picture treated in [35], where the product of functions was specified as the Moyal $\star$-product. That is, we have the following:

Proposition 3.26. [41] *If $f, g \in \mathcal{S}(\mathbb{R}^2)$, then*

$$\mathcal{F}(f \star_\Theta g) = (\mathcal{F}f) \diamond_\Theta (\mathcal{F}g), \tag{3.20}$$

where the product $f \star_\Theta g \in \mathcal{S}(\mathbb{R}^2)$ is defined by

$$(f \star_\Theta g)(\mathbf{x}) \coloneqq \frac{1}{2\pi\theta} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} f(\mathbf{x}+\mathbf{s}) g(\mathbf{x}+\mathbf{t}) e^{-i\langle \mathbf{s},\mathbf{t}\rangle_{\Theta^{-1}}} \, \mathrm{d}\mathbf{s}\, \mathrm{d}\mathbf{t}, \quad \mathbf{x} \in \mathbb{R}^2. \tag{3.21}$$

In the following, we let $f_{0,0} \in \mathcal{S}(\mathbb{R}^2)$ denote the Gaussian function defined by the expression

$$f_{0,0}(\mathbf{x}) := \frac{\theta}{\pi} e^{-\frac{\theta|\mathbf{x}|^2}{2}}, \quad \text{for } \mathbf{x} \in \mathbb{R}^2.$$

Remark 3.27. We have that $f_{0,0} \diamond_\Theta f_{0,0} = f_{0,0}$.

Furthermore, since we are in the Fourier dual picture, the "differentiation" operators we must consider are instead the coordinate operators.

In the following, for $s > 0$, we define the *Bessel-weighted L_2-space* by

$$L_2^s(\mathbb{R}^2) := \big\{ f \in L_2(\mathbb{R}^2) \, : \langle \cdot \rangle^s f \in L_2(\mathbb{R}^2) \big\}.$$

Definition 3.28. We denote by Q_1, Q_2 the *coordinate operators*, defined by the expression

$$(Q_k f)(\mathbf{x}) := x_k f(\mathbf{x}), \quad \text{for } f \in C^\infty_{\mathrm{com}}(\mathbb{R}^2),\ \mathbf{x} \in \mathbb{R}^2,\ k = 1, 2.$$

Both Q_1, Q_2 are essentially self-adjoint operators on $L_2(\mathbb{R}^2)$ whose closures are defined on the domain [76, pp. 53-54]

$$\mathrm{dom}(Q_k) := \Big\{ f \in L_2(\mathbb{R}^2) \, : \int_{\mathbb{R}^2} \big|t_k f(\mathbf{t})\big|^2 \, \mathrm{d}\mathbf{t} < \infty \Big\}, \quad k = 1, 2.$$

Hence, for each $k = 1, 2$, any subset of $\mathrm{dom}(Q_k)$ containing $C^\infty_{\mathrm{com}}(\mathbb{R}^2)$ is a core for Q_k (this includes Schwartz space $\mathcal{S}(\mathbb{R}^2)$ and Bessel-weighted L_2-space $L_2^1(\mathbb{R}^d)$).

Furthermore, on $L_2^2(\mathbb{R}^d)$, we have that the commutator

$$[Q_j, Q_k] = 0, \quad j, k = 1, 2.$$

Additionally, for every $\mathbf{t} = (t_1, t_2) \in \mathbb{R}^2$, we have the commutators

$$[Q_1, U^\Theta_{\mathbf{t}}] = t_1 U^\Theta_{\mathbf{t}}, \quad [Q_2, U^\Theta_{\mathbf{t}}] = t_2 U^\Theta_{\mathbf{t}}, \tag{3.22}$$

which each extend to a bounded operator on $L_2(\mathbb{R}^2)$.

Definition 3.29. Define the *Laplace multiplication operator* Δ_Θ on $L_2(\mathbb{R}^2)$ by the expression

$$\Delta_\Theta := Q_1^2 + Q_2^2, \quad \mathrm{dom}(\Delta_\Theta) := L_2^2(\mathbb{R}^2).$$

Moreover, we define the *Dirac multiplication operator* on $\mathbb{C}^2 \otimes L_2(\mathbb{R}^2)$ by

$$\mathcal{Q} = \gamma_1 \otimes Q_1 + \gamma_2 \otimes Q_2, \qquad \mathrm{dom}(\mathcal{Q}) := \mathbb{C}^2 \otimes L_2^1(\mathbb{R}^2),$$

where γ_1, γ_2 are 2-dimensional gamma matrices (see Definition 2.5 in Section 2.2.2 above).

Remark 3.30. Note that Δ_Θ does not actually depend on the choice of Θ; this convention is only chosen to distinguish the Laplace multiplication operator from the classical Laplacian. Since $\Delta_\Theta = \mathcal{F}(-\Delta)\mathcal{F}^{-1}$, the operator Δ_Θ is positive and self-adjoint, and since $\mathcal{Q} = (\mathbb{I}\otimes\mathcal{F})\mathcal{D}(\mathbb{I}\otimes\mathcal{F}^{-1})$, the operator $\mathcal{Q}$ is self-adjoint and, on the domain $\mathbb{C}^2\otimes L_2^2(\mathbb{R}^2)$, we have that $\mathcal{Q}^2 = \mathbb{I}\otimes\Delta_\Theta$.

Definition 3.31. Let $L_1(\mathbb{R}^2_\Theta)$ denote the trace class of $L_\infty(\mathbb{R}^2_\Theta)$ with respect to τ, which is equipped with the corresponding norm

$$\|X\|_1 \coloneqq \tau\big(|X|\big), \quad X\in L_1(\mathbb{R}^2_\Theta).$$

For $X\in L_1(\mathbb{R}^2_\Theta)$, if $\mathcal{C}\subset L_2(\mathbb{R}^2)$ is a core of Q_k and $X(\mathcal{C})\subset\mathcal{C}$, denote by $\eth_k X \coloneqq [Q_k, X]$ the (possibly unbounded) commutator of Q_k with X defined on $\mathcal{C}$, for each $k=1,2$. If $\eth_k X$ extends to a bounded operator, then $\eth_k X\in L_\infty(\mathbb{R}^d_\Theta)$ [53, Proposition 6.12]. For $m\in\mathbb{N}$, we define the *noncommutative Sobolev space* $W_1^m(\mathbb{R}^2_\Theta)$ by

$$W_1^m(\mathbb{R}^2_\Theta) \coloneqq \big\{X\in L_1(\mathbb{R}^2_\Theta)\ :\eth_1^{\alpha_1}\eth_2^{\alpha_2}X\in L_1(\mathbb{R}^2_\Theta),\ \forall\alpha_1,\alpha_2\in\mathbb{N}\text{ s.t. }\alpha_1+\alpha_2\le m\big\},$$

and equip this space with the norm

$$\|X\|_{W_1^m} \coloneqq \sum_{\alpha_1+\alpha_2\le m}\|\eth_1^{\alpha_1}\eth_2^{\alpha_2}X\|_1, \quad \text{for } X\in W_1^m(\mathbb{R}^2_\Theta).$$

Remark 3.32. By [86, Lemma 3.3], the subspace $\mathcal{S}(\mathbb{R}^2_\Theta)$ is dense in $W_1^2(\mathbb{R}^2_\Theta)$.

We have the following noncommutative analogue of a Cwikel estimate, whose proof may be found in [53]. We let $\nabla_\Theta \coloneqq (Q_1, Q_2)$, so that

$$\langle\nabla_\Theta\rangle = (1+Q_1^2+Q_2^2)^{\frac12} = (1+\Delta_\Theta)^{\frac12}.$$

Note that ∇_Θ, like Δ_Θ, does not depend upon the choice of Θ.

Theorem 3.33. [53, Theorems 7.6 and 7.7] *If $\varepsilon>0$ and $X\in W_1^2(\mathbb{R}^2_\Theta)$, then*

$$X\langle\nabla_\Theta\rangle^{-2}\in\mathcal{L}_{1,\infty}, \quad X\langle\nabla_\Theta\rangle^{-2-\varepsilon}\in\mathcal{L}_1,$$

and

$$\big\|X\langle\nabla_\Theta\rangle^{-2}\big\|_{1,\infty} \le \text{const}\cdot\|X\|_{W_1^2}.$$

3.4.2 The algebra of rapidly decreasing double-sequences

In this section, we shall investigate the noncommutative algebraic structure of the Fréchet algebra $\big(\mathcal{S}(\mathbb{R}^2),\diamond_\Theta\big)$ to demonstrate that it is closed under taking positive real powers. This is done by recalling the algebra of rapidly decreasing double-sequences of J. Gracia-Bondía and J. Várilly [41].

Definition 3.34. We say that a square-summable double sequence $c = \{c_{m,n}\}_{m,n\in\mathbb{N}} \in \ell_2(\mathbb{N}^2)$ is *rapidly decreasing* if, for every $k \in \mathbb{N}$,

$$r_k(c) := \Big(\sum_{m,n\in\mathbb{N}} (m+1)^{2k}(n+1)^{2k}|c_{m,n}|^2\Big)^{\frac{1}{2}} < \infty.$$

The space of rapidly decreasing double sequences, denoted by $\mathbf{S} \subset \ell_2(\mathbb{N}^2)$, equipped with the family of seminorms $\{r_k\}_{k\in\mathbb{N}}$ forms a Fréchet space [41]. In addition, we equip this space with the *matrix product*, which we define by the expression

$$c \cdot d := \Big\{ \sum_{j\in\mathbb{N}} c_{m,j}d_{j,n}\Big\}_{m,n\in\mathbb{N}}, \quad c, d \in \mathbf{S}.$$

Remark 3.35. We have

$$r_k(c \cdot d) \leq r_k(c)r_k(d).$$

In particular, $\mathbf{S}$ equipped with the matrix product is a Fréchet algebra.

Proof. Suppose $c, d \in \mathbf{S}$, and let $k \in \mathbb{N}$. By the triangle inequality and the Hölder inequality, we observe that

$$\Big|\sum_{j\in\mathbb{N}} c_{m,j}d_{j,n}\Big| \leq \Big(\sum_{j\in\mathbb{N}} |c_{m,j}|^2\Big)^{\frac{1}{2}}\Big(\sum_{j\in\mathbb{N}} |d_{j,n}|^2\Big)^{\frac{1}{2}},$$

so that

$$r_k(c \cdot d)^2 \leq \Big(\sum_{m,j\in\mathbb{N}} (m+1)^{2k}|c_{m,j}|^2\Big)\Big(\sum_{j,n\in\mathbb{N}} (n+1)^{2k}|d_{j,n}|^2\Big).$$

Hence, $r_k(c \cdot d) \leq r_k(c)r_k(d)$, □

We identify the algebra $\mathbf{S}$ with the corresponding space of bounded operators on the Hilbert space $\ell_2(\mathbb{N})$ defined via the action

$$c\mathbf{x} := \Big\{ \sum_{j\in\mathbb{N}} c_{m,j}x_j\Big\}_{m\in\mathbb{N}}, \quad c = \{c_{m,n}\}_{m,n\in\mathbb{N}} \in \mathbf{S},\ \mathbf{x} = \{x_j\}_{j\in\mathbb{N}} \in \ell_2(\mathbb{N}).$$

The matrix product therefore corresponds to the composition product of operators. Moreover, the theory of bounded operators on $\ell_2(\mathbb{N})$ provides a natural means of defining positivity of elements of $\mathbf{S}$, as well as the continuous functional calculus.

Lemma 3.36. *If* $0 \leq c \in \mathbf{S}$, *then* $c^p \in \mathbf{S}$ *for all* $p > 0$.

Proof. Firstly, we prove the assertion for $p = \frac{1}{2}$. Let $d = c^{\frac{1}{2}}$. Since d is self-adjoint, we observe that

$$\begin{aligned}|d_{m,n}|^2 = \big|\langle d\mathbf{e}_m, \mathbf{e}_n\rangle\big|\big|\langle \mathbf{e}_m, d\mathbf{e}_n\rangle\big| \leq \|d\mathbf{e}_m\|_2\|d\mathbf{e}_n\|_2 &= \big|\langle d^2\mathbf{e}_m, \mathbf{e}_m\rangle\big|^{\frac{1}{2}}\big|\langle d^2\mathbf{e}_n, \mathbf{e}_n\rangle\big|^{\frac{1}{2}} \\ &= |c_{m,m}|^{\frac{1}{2}}|c_{n,n}|^{\frac{1}{2}},\end{aligned}$$

where the vectors $\{\mathbf{e}_j\}_{j=0}^{\infty}$ are the standard basis vectors for $\ell_2(\mathbb{N})$. Consequently, for $k \in \mathbb{N}$, we have that

$$\begin{aligned} r_k(d)^2 &= \sum_{m,n=0}^{\infty} (m+1)^{2k}(n+1)^{2k}|d_{m,n}|^2 \\ &\leq \sum_{m,n=0}^{\infty} (m+1)^{2k}(n+1)^{2k}|c_{m,m}|^{\frac{1}{2}}|c_{n,n}|^{\frac{1}{2}} = \left(\sum_{m=0}^{\infty}(m+1)^{2k}|c_{m,m}|^{\frac{1}{2}}\right)^2. \end{aligned}$$

By applying the Hölder inequality, we obtain

$$\sum_{m=0}^{\infty}(m+1)^{2k}|c_{m,m}|^{\frac{1}{2}} \leq \left(\sum_{m=0}^{\infty}\frac{1}{(m+1)^{\frac{8}{3}}}\right)^{\frac{3}{4}}\left(\sum_{m=0}^{\infty}(m+1)^{8k+8}|c_{m,m}|^2\right)^{\frac{1}{4}}.$$

Therefore, we have

$$r_k(d)^2 \leq \mathrm{const}\cdot r_{2k+2}(c).$$

In particular, $r_k(d)$ is finite for every $k \in \mathbb{N}$. This proves the assertion for $p = \frac{1}{2}$.

By induction, the assertion holds for $p = 2^{-n}$, $n \in \mathbb{N}$.

Let $p > \frac{1}{2}$. Since c, c^p are self-adjoint, we have that

$$\left|(c^p)_{m,n}\right|^2 \leq \|c^p\mathbf{e}_m\|\|c^p\mathbf{e}_n\| \leq \|c\|_\infty^{2p-1}\cdot\|c^{\frac{1}{2}}\mathbf{e}_m\|\|c^{\frac{1}{2}}\mathbf{e}_n\| \leq \|c\|_\infty^{2p-1}\cdot|c_{m,m}|^{\frac{1}{2}}|c_{n,n}|^{\frac{1}{2}}.$$

Therefore,

$$\begin{aligned} r_k(c^p) &\leq \|c\|_\infty^{2p-1}\sum_{m,n\in\mathbb{N}}(m+1)^{2k}(n+1)^{2k}|c_{m,m}|^{\frac{1}{2}}\cdot|c_{n,n}|^{\frac{1}{2}} \\ &= \|c\|_\infty^{2p-1}\left(\sum_{m=0}^{\infty}(m+1)^{2k}|c_{m,m}|^{\frac{1}{2}}\right)^2. \end{aligned}$$

That is,

$$r_k(c^p) \leq \mathrm{const}\cdot\|c\|_\infty^{2p-1}r_{2k+2}(c)^{\frac{1}{2}}.$$

This proves the assertion for $p > \frac{1}{2}$. By considering $c^p = (c^{2^{-n}})^{2^n p}$, where $2^n p > 1$, we conclude the argument for $p > 0$. □

Remark 3.37. If $c \in \mathbf{S}$, then $c^2 \in \mathbf{S}$ and, by Lemma 3.36, $|c| = (c^2)^{\frac{1}{2}} \in \mathbf{S}$. However, $c = |c| - \big(|c| - c\big)$. Hence, $\mathbf{S}$ is spanned by $\mathbf{S}_+$.

By Proposition 3.26, the work done for the Fréchet algebra $\big(\mathcal{S}(\mathbb{R}^2), \star_\Theta\big)$ in [41] applies equivalently to $\big(\mathcal{S}(\mathbb{R}^2), \diamond_\Theta\big)$ (see also [35]). Define a family of functions $f_{m,n} \in \mathcal{S}(\mathbb{R}^2)$, for $m, n \in \mathbb{N}$, as follows: for $\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2$, let

$$f_{m,n}(\mathbf{x}) := \begin{cases} \sqrt{\dfrac{n!}{m!}}\big(i\sqrt{\theta}(x_1 - ix_2)\big)^{m-n}\mathrm{L}_n^{(m-n)}\big(\theta|\mathbf{x}|^2\big)f_{0,0}(\mathbf{x}), & \text{if } m \geq n, \\ \sqrt{\dfrac{m!}{n!}}\big(i\sqrt{\theta}(x_1 + ix_2)\big)^{n-m}\mathrm{L}_m^{(n-m)}\big(\theta|\mathbf{x}|^2\big)f_{0,0}(\mathbf{x}), & \text{otherwise,} \end{cases} \tag{3.23}$$

where $\mathrm{L}_n^{(\alpha)}$ denotes the nth Laguerre polynomial with parameter α.

Remark 3.38. For every $m, n, k, \ell \in \mathbb{N}$,

$$f_{m,n} \diamond_\Theta f_{k,\ell} = \delta_{n,k} f_{m,\ell},$$

where $\delta_{m,n}$ denotes the Kronecker delta, since the family $\{f_{m,n}\}_{m,n}$ consists of the Fourier transforms (up to constant factors) of the oscillator basis functions of $\mathcal{S}(\mathbb{R}^2)$ found in [35, §8.1].

Proposition 3.39. [41, Theorem 6], [35, Proposition 2.5] *For every $g \in \mathcal{S}(\mathbb{R}^2)$ and every $m, n \in \mathbb{N}$, there exists some $c_{m,n}(g) \in \mathbb{C}$ such that*

$$(f_{m,m} \diamond_\Theta g \diamond_\Theta f_{n,n})(\mathbf{x}) = c_{m,n}(g) f_{m,n}(\mathbf{x}), \quad \textit{for all } \mathbf{x} \in \mathbb{R}^2, \tag{3.24}$$

where the double sequence $\big\{c_{m,n}(g)\big\}_{m,n\in\mathbb{N}}$ belongs to $\mathbf{S}$. Moreover, the map $\Xi : \mathcal{S}(\mathbb{R}^2_\Theta) \to \mathbf{S}$ defined by

$$\Xi\big[\mathrm{Op}_\Theta(g)\big] \coloneqq \big\{c_{m,n}(g)\big\}_{m,n\in\mathbb{N}}, \quad g \in \mathcal{S}(\mathbb{R}^2),$$

is a Fréchet algebra $*$-isomorphism between $\mathcal{S}(\mathbb{R}^2_\Theta)$ and $\mathbf{S}$.

Remark 3.40. Recall τ denotes the normal trace on $L_\infty(\mathbb{R}^2_\Theta)$. By Remarks 3.25 and 3.38, we have that

$$\mathrm{Op}_\Theta(f_{m,n})^2 = \delta_{m,n}\, \mathrm{Op}_\Theta(f_{m,n}), \quad \text{for all } m, n \in \mathbb{N}.$$

Hence, $\mathrm{Op}_\Theta(f_{m,n})$ is nilpotent whenever $m \neq n$, in which case $\tau\big(\mathrm{Op}_\Theta(f_{m,n})\big) = 0$; otherwise, $\mathrm{Op}_\Theta(f_{m,m})$ is a projection. In fact, by (3.24) above, we have that

$$\mathrm{Op}_\Theta(f_{m,m})\, \mathrm{Op}_\Theta(g)\, \mathrm{Op}_\Theta(f_{m,m}) = c_{m,m}(g)\, \mathrm{Op}_\Theta(f_{m,m}), \quad \text{for all } g \in \mathcal{S}(\mathbb{R}^2),$$

so $\mathrm{Op}_\Theta(f_{m,m})$ is an atom, and so $\tau\big(\mathrm{Op}_\Theta(f_{m,m})\big) = 1$ by normality of τ. Therefore, since $f_{m,n}(\mathbf{0}) = \frac{\theta}{\pi}\delta_{m,n}$, for all $m, n \in \mathbb{N}$, we have that

$$\tau\big(\mathrm{Op}_\Theta(f_{m,n})\big) = \delta_{m,n} = \frac{\pi}{\theta} f_{m,n}(\mathbf{0}), \quad \text{for all } m, n \in \mathbb{N},$$

where we denoted $\mathbf{0} = (0, 0) \in \mathbb{R}^2$. Therefore, by continuity and linearity of τ, and since $\{f_{m,n}\}_{m,n\in\mathbb{N}}$ is an orthogonal basis for $\mathcal{S}(\mathbb{R}^2)$, we observe that

$$\tau\big(\mathrm{Op}_\Theta(g)\big) = \sum_{m,n\in\mathbb{N}} c_{m,n}(g)\tau\big(\mathrm{Op}_\Theta(f_{m,n})\big) = \frac{\pi}{\theta} \sum_{m,n\in\mathbb{N}} c_{m,n}(g) f_{m,n}(\mathbf{0}) = \frac{\pi}{\theta} g(\mathbf{0}), \tag{3.25}$$

for all $g \in \mathcal{S}(\mathbb{R}^2)$.

Remark 3.41. Let $\Xi : \mathcal{S}(\mathbb{R}^2_\Theta) \to \mathbf{S}$ be the Fréchet algebra $*$-isomorphism from Proposition 3.39 above. Then, for every $X \in \mathcal{S}(\mathbb{R}^2_\Theta)$, there exists a double-sequence $c_X \in \mathbf{S}$ such that $\Xi[X] = c_X$. If $n \in \mathbb{N}$, then

$$X^n = \big(\Xi^{-1}[c_X]\big)^n = \Xi^{-1}\big[c_X^n\big] \in \mathcal{S}(\mathbb{R}^2_\Theta)$$

since Ξ^{-1} is an algebra isomorphism. Therefore, since every continuous function is approximated by polynomials, and since Ξ is continuous, the continuous functional calculus on $\mathbf{S}$ is preserved by Ξ. In particular, if $f \in \mathcal{S}(\mathbb{R}^2)$, then the double sequence $\{c_{m,n}(f)\}_{m,n\in\mathbb{N}} \in \mathbf{S}$ defines a positive operator on $\ell_2(\mathbb{N})$ if and only if $\mathrm{Op}_\Theta(f) \in \mathcal{S}(\mathbb{R}^2_\Theta)$ is a positive operator on $L_2(\mathbb{R}^2)$.

Corollary 3.42. *If f is a Schwartz function on $\mathbb{R}^2$ such that $\mathrm{Op}_\Theta(f)$ is a positive operator, then $\big(\mathrm{Op}_\Theta(f)\big)^p \in \mathcal{S}(\mathbb{R}^2_\Theta)$, for every $p > 0$. In particular, for every $p > 0$, there exists some $f_p \in \mathcal{S}(\mathbb{R}^2)$ such that*

$$\big(\mathrm{Op}_\Theta(f)\big)^p = \mathrm{Op}_\Theta(f_p).$$

Proof. By Remark 3.41, the isomorphism $\Xi : \mathcal{S}(\mathbb{R}^2_\Theta) \to \mathbf{S}$ preserves the continuous functional calculus. Hence, for $p > 0$, Lemma 3.36 implies that

$$X^p = \big(\Xi^{-1}[c_X]\big)^p = \Xi^{-1}[c_X^p] \in \mathcal{S}(\mathbb{R}^2_\Theta), \quad \text{whenever } 0 \le X \in \mathcal{S}(\mathbb{R}^2_\Theta).$$

By construction of $\mathcal{S}(\mathbb{R}^2_\Theta)$, since $X \in \mathcal{S}(\mathbb{R}^2_\Theta)$, there exists some Schwartz function $f \in \mathcal{S}(\mathbb{R}^2)$ such that $X = \mathrm{Op}_\Theta(f)$. Likewise, for every $p > 0$, since $X^p \in \mathcal{S}(\mathbb{R}^2_\Theta)$, there exists some $f_p \in \mathcal{S}(\mathbb{R}^2)$ such that $X^p = \mathrm{Op}_\Theta(f_p)$. $\square$

3.4.3 Application of residue formula to the Moyal plane

In this section, we verify that the conditions of Theorem 1.1 are satisfied by the operators on $L_2(\mathbb{R}^2)$ given by

$$A := \mathrm{Op}_\Theta(f) \quad \text{and} \quad B := \langle\nabla_\Theta\rangle^{-2} = (1 + \Delta_\Theta)^{-1},$$

for $f \in \mathcal{S}(\mathbb{R}^2)$ such that $\mathrm{Op}_\Theta(f) \ge 0$, and calculate the value of the trace $\mathrm{Tr}(B^{1+\varepsilon}A^{1+\varepsilon})$, for $\varepsilon > 0$.

Firstly, we verify that the commutator $[A^{\frac{1}{2}}, B] \in \mathcal{L}_1$.

Lemma 3.43. *If $f \in \mathcal{S}(\mathbb{R}^2)$, then*

$$\big[\mathrm{Op}_\Theta(f), \langle\nabla_\Theta\rangle^{-2}\big] \in \mathcal{L}_1.$$

Proof. For simplicity, it suffices to work over the domain $\mathcal{S}(\mathbb{R}^2)$, which is a core of Δ_Θ and invariant under action of $\mathrm{Op}_\Theta(f)$. By Lemma 2.2 (i), we have that

$$\big[\mathrm{Op}_\Theta(f), \langle\nabla_\Theta\rangle^{-2}\big] \overset{(2.1)}{=} -\langle\nabla_\Theta\rangle^{-2}\big[\mathrm{Op}_\Theta(f), \langle\nabla_\Theta\rangle^{2}\big]\langle\nabla_\Theta\rangle^{-2} = \langle\nabla_\Theta\rangle^{-2}\big[\Delta_\Theta, \mathrm{Op}_\Theta(f)\big]\langle\nabla_\Theta\rangle^{-2},$$

where in the last line we used the fact that the identity operator on $L_2(\mathbb{R}^2)$ commutes with $\mathrm{Op}_\Theta(f)$. By (3.22), we have for each $k = 1, 2$ that

$$\big[Q_k, \mathrm{Op}_\Theta(f)\big] \overset{(3.19)}{=} \int_{\mathbb{R}^2} f(\mathbf{t})[Q_k, U_{\mathbf{t}}^\Theta]\,\mathrm{d}\mathbf{t} \overset{(3.22)}{=} \int_{\mathbb{R}^2} t_k f(\mathbf{t}) U_{\mathbf{t}}^\Theta\,\mathrm{d}\mathbf{t} = \int_{\mathbb{R}^2} (Q_k f)(\mathbf{t}) U_{\mathbf{t}}^\Theta\,\mathrm{d}\mathbf{t}$$
$$= \mathrm{Op}_\Theta(Q_k f).$$

Moreover, since $\Delta_\Theta = Q_1^2 + Q_2^2$ by definition, we have that

$$\begin{aligned}\big[\Delta_\Theta, \mathrm{Op}_\Theta(f)\big] &= \big[Q_1^2 + Q_2^2, \mathrm{Op}_\Theta(f)\big]\\ &= Q_1\big[Q_1, \mathrm{Op}_\Theta(f)\big] + Q_2\big[Q_2, \mathrm{Op}_\Theta(f)\big] + \big[Q_1, \mathrm{Op}_\Theta(f)\big]Q_1 + \big[Q_2, \mathrm{Op}_\Theta(f)\big]Q_2\\ &= Q_1 \mathrm{Op}_\Theta(Q_1 f) + Q_2 \mathrm{Op}_\Theta(Q_2 f) + \mathrm{Op}_\Theta(Q_1 f)Q_1 + \mathrm{Op}_\Theta(Q_2 f)Q_2,\end{aligned}$$

on the dense domain $\mathcal{S}(\mathbb{R}^2)$. Therefore, we have that

$$\begin{aligned}&\big[\mathrm{Op}_\Theta(f), \langle\nabla_\Theta\rangle^{-2}\big]\\ &\quad= Q_1\langle\nabla_\Theta\rangle^{-1} \cdot \langle\nabla_\Theta\rangle^{-1} \mathrm{Op}_\Theta(Q_1 f)\langle\nabla_\Theta\rangle^{-2} + Q_2\langle\nabla_\Theta\rangle^{-1} \cdot \langle\nabla_\Theta\rangle^{-1} \mathrm{Op}_\Theta(Q_2 f)\langle\nabla_\Theta\rangle^{-2}\\ &\qquad+ \langle\nabla_\Theta\rangle^{-2} \mathrm{Op}_\Theta(Q_1 f)\langle\nabla_\Theta\rangle^{-1} \cdot Q_1\langle\nabla_\Theta\rangle^{-1} + \langle\nabla_\Theta\rangle^{-2} \mathrm{Op}_\Theta(Q_2 f)\langle\nabla_\Theta\rangle^{-1} \cdot Q_2\langle\nabla_\Theta\rangle^{-1},\end{aligned}$$

which extends to a bounded operator on $L_2(\mathbb{R}^2)$ by the spectral theorem. Hence,

$$\begin{aligned}\Big\|\big[\mathrm{Op}_\Theta(f), \langle\nabla_\Theta\rangle^{-2}\big]\Big\|_1 &\le \big\|\langle\nabla_\Theta\rangle^{-1} \mathrm{Op}_\Theta(Q_1 f)\langle\nabla_\Theta\rangle^{-2}\big\|_1 + \big\|\langle\nabla_\Theta\rangle^{-1} \mathrm{Op}_\Theta(Q_2 f)\langle\nabla_\Theta\rangle^{-2}\big\|_1\\ &\quad+ \big\|\langle\nabla_\Theta\rangle^{-2} \mathrm{Op}_\Theta(Q_1 f)\langle\nabla_\Theta\rangle^{-1}\big\|_1 + \big\|\langle\nabla_\Theta\rangle^{-2} \mathrm{Op}_\Theta(Q_2 f)\langle\nabla_\Theta\rangle^{-1}\big\|_1\\ &\overset{(2.11)}{\le} 2\big\|\mathrm{Op}_\Theta(Q_1 f)\langle\nabla_\Theta\rangle^{-3}\big\|_1 + 2\big\|\mathrm{Op}_\Theta(Q_2 f)\langle\nabla_\Theta\rangle^{-3}\big\|_1.\end{aligned}$$

where in the last line we used Theorem 2.20. The assertion now follows from Theorem 3.33 (with $\varepsilon = \frac{1}{2}$). □

Furthermore, we obtain the following expression for the classical trace of $AB^{1+\varepsilon}$.

Lemma 3.44. *If $f \in \mathcal{S}(\mathbb{R}^2)$ and if $\varepsilon > 0$, then*

$$\mathrm{Tr}\,\big(\langle\nabla_\Theta\rangle^{-2(1+\varepsilon)} \mathrm{Op}_\Theta(f)\big) = \frac{\pi}{\varepsilon} f(\mathbf{0}).$$

Proof. Appealing to Remark 3.24, $\langle\nabla_\Theta\rangle^{-2(1+\varepsilon)} \mathrm{Op}_\Theta(f)$ is an integral operator on $L_2(\mathbb{R}^2)$ whose integral kernel is defined by the expression

$$K(\mathbf{x}, \mathbf{t}) = \langle\mathbf{x}\rangle^{-2(1+\varepsilon)} f(\mathbf{x} - \mathbf{t}) e^{i\langle\mathbf{t},\mathbf{x}\rangle_\Theta}, \quad \mathbf{x}, \mathbf{t} \in \mathbb{R}^2.$$

By Theorem 3.33, this operator belongs to $\mathcal{L}_1$. Moreover, since the integral kernel K is continuous and belongs to $L_2(\mathbb{R}^2 \times \mathbb{R}^2)$, Proposition 2.32 implies that

$$\mathrm{Tr}\,\big(\langle\nabla_\Theta\rangle^{-2(1+\varepsilon)} \mathrm{Op}_\Theta(f)\big) = \int_{\mathbb{R}^2} \langle\mathbf{t}\rangle^{-2(1+\varepsilon)} f(\mathbf{0}) e^{i\langle\mathbf{t},\mathbf{t}\rangle_\Theta}\,\mathrm{d}\mathbf{t} = f(\mathbf{0}) \cdot \int_{\mathbb{R}^2} \langle\mathbf{t}\rangle^{-2(1+\varepsilon)}\,\mathrm{d}\mathbf{t}.$$

The integral on the right-hand side is precisely $\frac{\pi}{\varepsilon}$, and we are done. □

Using these results, we arrive at the main result of this section.

Proposition 3.45. *If $f \in \mathcal{S}(\mathbb{R}^2)$, then $\mathrm{Op}_\Theta(f)\langle\nabla_\Theta\rangle^{-2}$ is a Dixmier measurable operator and, for any extended limit ω,*

$$\mathrm{Tr}_\omega\left(\mathrm{Op}_\Theta(f)\langle\nabla_\Theta\rangle^{-2}\right) = \pi f(\mathbf{0}).$$

Proof. Firstly, denote $A \coloneqq \mathrm{Op}_\Theta(f)$. Recalling Remark 3.37, we may assume without loss of generality that $A \geq 0$. Then, by Corollary 3.42, there exists some $g \in \mathcal{S}(\mathbb{R}^2)$ such that $A^{\frac{1}{2}} = \mathrm{Op}_\Theta(g)$. Setting $B \coloneqq \langle\nabla_\Theta\rangle^{-2}$, we infer from Lemma 3.43 that $[A^{\frac{1}{2}}, B] \in \mathcal{L}_1$.

Moreover, by Corollary 3.42, there exists some Schwartz function $f_{1+\varepsilon} \in \mathcal{S}(\mathbb{R}^2)$ such that $A^{1+\varepsilon} = \mathrm{Op}_\Theta(f_{1+\varepsilon})$. By Remark 3.40 and Lemma 3.44, we have

$$\varepsilon\,\mathrm{Tr}(B^{1+\varepsilon}A^{1+\varepsilon}) = \pi f_{1+\varepsilon}(\mathbf{0}) = \theta\tau(\mathrm{Op}_\Theta(f_{1+\varepsilon})) = \theta\tau(A^{1+\varepsilon}).$$

Hence, by [34, Theorem 3.6], we have the limit

$$\lim_{\varepsilon\downarrow 0}\varepsilon\,\mathrm{Tr}(B^{1+\varepsilon}A^{1+\varepsilon}) = \theta\lim_{\varepsilon\downarrow 0}\tau(A^{1+\varepsilon}) = \theta\tau(A) = \pi f(\mathbf{0}).$$

Therefore, since $[A^{\frac{1}{2}}, B] \in \mathcal{L}_1$, and since $AB \in \mathcal{L}_{1,\infty}$ by Theorem 3.33, it follows from Theorem 3.7 that

$$\mathrm{Tr}_\omega(AB) = \lim_{\varepsilon\downarrow 0}\varepsilon\,\mathrm{Tr}(B^{1+\varepsilon}A^{1+\varepsilon}) = \pi f(\mathbf{0}). \qquad \square$$

Note that if we let $f = \mathcal{F}h$ in Proposition 3.45, for $h \in \mathcal{S}(\mathbb{R}^2)$, then

$$\int_{\mathbb{R}^2} h(\mathbf{t})\,\mathrm{d}\mathbf{t} = 2\pi(\mathcal{F}h)(\mathbf{0}) = 2\,\mathrm{Tr}_\omega\left(\mathrm{Op}_\Theta(\mathcal{F}h)\langle\nabla_\Theta\rangle^{-2}\right).$$

Using the noncommutative Cwikel estimate (see Theorem 3.33 above), Proposition 3.45 may be easily extended to noncommutative Sobolev space.

Corollary 3.46. *If $X \in W_1^2(\mathbb{R}^2_\Theta)$, then $(\mathbb{I}\otimes X)\langle\mathcal{Q}\rangle^{-2}$ is a Dixmier measurable operator on $\mathbb{C}^2 \otimes L_2(\mathbb{R}^2)$ and, for any extended limit ω,*

$$\mathrm{Tr}_\omega\left((\mathbb{I}\otimes X)\langle\mathcal{Q}\rangle^{-2}\right) = 2\theta\tau(X).$$

Proof. Since $(\mathbb{I}\otimes X)\langle\mathcal{Q}\rangle^{-2} = \mathbb{I}\otimes X\langle\nabla_\Theta\rangle^{-2}$, it suffices to check that

$$\mathrm{Tr}_\omega\left(X\langle\nabla_\Theta\rangle^{-2}\right) = \theta\tau(X).$$

By Remark 3.32, there exists a sequence $\{f_n\}_{n\in\mathbb{N}} \subset \mathcal{S}(\mathbb{R}^2)$ such that $\mathrm{Op}_\Theta(f_n) \to X$ in the norm-induced topology of $W_1^2(\mathbb{R}^2_\Theta)$ as $n \to \infty$. In particular, since $\mathrm{Op}_\Theta(f_n) \to X$

as $n \to \infty$ in the L_1-norm, we also have that $\tau\big(\mathrm{Op}_\Theta(f_n)\big) \to \tau(X)$ as $n \to \infty$. By Theorem 3.33, we have

$$\Big\| X\langle\nabla_\Theta\rangle^{-2} - \mathrm{Op}_\Theta(f_n)\langle\nabla_\Theta\rangle^{-2}\Big\|_{1,\infty} \leq \mathrm{const}\cdot \big\|X - \mathrm{Op}_\Theta(f_n)\big\|_{W_1^2} \to 0.$$

Hence, the sequence of operators $\big\{\mathrm{Op}_\Theta(f_n)\langle\nabla_\Theta\rangle^{-2}\big\}_{n\in\mathbb{N}} \subset \mathcal{L}_{1,\infty}$ converges to $X\langle\nabla_\Theta\rangle^{-2}$ in the topology induced by the $\mathcal{L}_{1,\infty}$-quasi-norm. Therefore, since Tr_ω is continuous in $\mathcal{L}_{1,\infty}$,

$$\begin{aligned}\mathrm{Tr}_\omega\left(X\langle\nabla_\Theta\rangle^{-2}\right) = \lim_{n\to\infty} \mathrm{Tr}_\omega\left(\mathrm{Op}_\Theta(f_n)\langle\nabla_\Theta\rangle^{-2}\right) = \lim_{n\to\infty} \pi f_n(\mathbf{0}) &\overset{(3.25)}{=} \theta \lim_{n\to\infty} \tau\big(\mathrm{Op}_\Theta(f_n)\big) \\ &= \theta\tau(X)\end{aligned}$$

where in the second equality we appealed to Proposition 3.45. □

4

Lipschitz-type estimates for the electromagnetic Dirac operator on $\mathbb{R}^d$

In the present chapter, we prove Theorems 1.2 and 1.9. As was already explained in Section 1.2.2 above, Theorem 1.2 follows from Theorem 1.9 using the techniques of double operator integration. Namely, we can show (see Section 4.2 below for details) that for $f \in C^\infty(\mathbb{R})$ with $0 \leq f' \in \mathcal{S}(\mathbb{R})$, and the sufficiently well-behaved bounded potential

$$V = \mathbb{I} \otimes M_\phi - \sum_{j=1}^{d} \gamma_j \otimes M_{a_j},$$

we have

$$f(\mathcal{D}+V) - f(\mathcal{D}) \in \begin{cases} \mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) + \mathcal{L}_{\frac{d}{2}}, & \text{if } \mathbf{A} = 0 \text{ and } \phi \neq 0, \\ \mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) + \mathcal{L}_d, & \text{if } \mathbf{A} \neq 0. \end{cases}$$

Thus, the asymptotic behaviour of the singular values of the operator $f(\mathcal{D}+V) - f(\mathcal{D})$ is determined by that of the operator $\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})$. This makes investigating the behaviour of $\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})$ our primary objective in this chapter.

Using the integral representation

$$\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) = \frac{1}{\pi} \mathfrak{Re} \left(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}} \Big(\big(\mathcal{D}+V+i(1+\lambda)^{\frac{1}{2}}\big)^{-1} - \big(\mathcal{D}+i(1+\lambda)^{\frac{1}{2}}\big)^{-1} \Big) \right),$$

the second resolvent identity and Cwikel estimates, we can distinguish operators which can be neglected (modulo appropriate Schatten ideals) and write $\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})$ as an operator of the form $\sum_\alpha M_{\mathrm{F}_\alpha}\big(\mathbb{I} \otimes g_\alpha(\nabla)\big)$, where the operator $M_{\mathrm{F}_\alpha}\big(\mathbb{I} \otimes g_\alpha(\nabla)\big)$ belongs to the required weak Schatten ideal for every α ($\mathcal{L}_{\frac{d}{2}}$ for the electric case, and $\mathcal{L}_d$ for the magnetic case).

The contents of this chapter are the product of my work with co-authors in [52].

4.1 Lipschitz-type estimates for the smoothed signum of the Dirac operator

4.1.1 Auxiliary integral representation and Cwikel estimates

In the sequel, we shall make use of the notations

$$\mathcal{R}_{0,\lambda} := \big(\mathcal{D} + i(1+\lambda)^{\frac{1}{2}}\big)^{-1}, \quad \mathcal{R}_{1,\lambda} := \big(\mathcal{D} + V + i(1+\lambda)^{\frac{1}{2}}\big)^{-1}, \quad \lambda \geq 0. \tag{4.1}$$

We make several immediate observations. Note that

$$|\mathcal{R}_{0,\lambda}| = (1+\lambda+\mathcal{D}^2)^{-\frac{1}{2}} = \mathbb{I} \otimes (1+\lambda-\Delta)^{-\frac{1}{2}}. \tag{4.2}$$

By the spectral theorem, we have that

$$\|\mathcal{R}_{0,\lambda}\|_\infty,\ \|\mathcal{R}_{1,\lambda}\|_\infty \leq (1+\lambda)^{-\frac{1}{2}}.$$

Furthermore, by the second resolvent identity, we have that

$$\mathcal{R}_{1,\lambda} = \mathcal{R}_{0,\lambda} - \mathcal{R}_{1,\lambda} V \mathcal{R}_{0,\lambda}.$$

Hence, using this equality repeatedly, we obtain the following expressions:

$$\begin{aligned} \mathcal{R}_{1,\lambda} - \mathcal{R}_{0,\lambda} &= -\mathcal{R}_{1,\lambda} V \mathcal{R}_{0,\lambda} = \mathcal{R}_{1,\lambda}(V\mathcal{R}_{0,\lambda})^2 - \mathcal{R}_{0,\lambda} V \mathcal{R}_{0,\lambda} & (4.3) \\ &= -\mathcal{R}_{1,\lambda}(V\mathcal{R}_{0,\lambda})^3 + \mathcal{R}_{0,\lambda}(V\mathcal{R}_{0,\lambda})^2 - \mathcal{R}_{0,\lambda} V \mathcal{R}_{0,\lambda}. & (4.4) \end{aligned}$$

Proposition 4.1. *For any self-adjoint $V \in \mathcal{B}\big(\mathbb{C}^{N_d} \otimes L_2(\mathbb{R}^d)\big)$, we have*

$$\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) = \frac{1}{\pi} \mathfrak{Re}\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}} (\mathcal{R}_{1,\lambda} - \mathcal{R}_{0,\lambda})\Big), \tag{4.5}$$

where the integral on the right-hand side converges as a Bochner integral.

Proof. By [50, p. 282], we have

$$(1+A^2)^{-\frac{1}{2}} = \frac{1}{\pi}\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}(1+\lambda+A^2)^{-1},$$

for any self-adjoint operator A on $\mathcal{H}$. Hence, for all $\xi \in \mathbb{C}^{N_d} \otimes W_2^1(\mathbb{R}^d) = \mathrm{dom}(\mathcal{D}) = \mathrm{dom}(\mathcal{D}+V)$, we have

$$\big(\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})\big)\xi = \frac{1}{\pi}\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\Big((\mathcal{D}+V)\big(1+\lambda+(\mathcal{D}+V)^2\big)^{-1} - \mathcal{D}(1+\lambda+\mathcal{D}^2)^{-1}\Big)\xi.$$

Indeed, the integrand above defines a weak operator Lebesgue-integrable function on $(0,\infty)$; this follows from the fact that, for every $\xi,\eta\in\mathbb{C}^{N_d}\otimes L_2(\mathbb{R}^d)$, the map

$$\lambda\mapsto\frac{1}{\lambda^{\frac12}}\Big\langle(\mathcal{D}+V)\big(1+\lambda+(\mathcal{D}+V)^2\big)^{-1}\xi,\eta\Big\rangle-\frac{1}{\lambda^{\frac12}}\Big\langle\mathcal{D}(1+\lambda+\mathcal{D}^2)^{-1}\xi,\eta\Big\rangle,\quad\text{for }\lambda>0,$$

defines a Lebesgue-measurable function on $(0,\infty)$ and, by [19, Appendix A-Lemma 6 (2)], we have the estimate

$$\int_0^\infty\frac{\mathrm{d}\lambda}{\lambda^{\frac12}}\Big\|(\mathcal{D}+V)\big(1+\lambda+(\mathcal{D}+V)^2\big)^{-1}-\mathcal{D}(1+\lambda+\mathcal{D}^2)^{-1}\Big\|_\infty\le\int_0^\infty\frac{\|V\|_\infty\,\mathrm{d}\lambda}{\lambda^{\frac12}(1+\lambda)}<\infty.$$

Therefore, we may

$$\mathrm{g}(\mathcal{D}+V)-\mathrm{g}(\mathcal{D})=\frac{1}{\pi}\int_0^\infty\frac{\mathrm{d}\lambda}{\lambda^{\frac12}}\Big((\mathcal{D}+V)\big(1+\lambda+(\mathcal{D}+V)^2\big)^{-1}-\mathcal{D}(1+\lambda+\mathcal{D}^2)^{-1}\Big)$$

as a weak operator integral. In fact, one can get that this integral converges in the Bochner sense from continuity [36, Lemma 3.1]. Furthermore, since

$$\mathfrak{Re}(\mathcal{R}_{0,\lambda})=\mathcal{D}(1+\lambda+\mathcal{D}^2)^{-1},\quad\mathfrak{Re}(\mathcal{R}_{1,\lambda})=(\mathcal{D}+V)\big(1+\lambda+(\mathcal{D}+V)^2\big)^{-1},$$

we have that

$$\mathrm{g}(\mathcal{D}+V)-\mathrm{g}(\mathcal{D})=\frac{1}{\pi}\,\mathfrak{Re}\Big(\int_0^\infty\frac{\mathrm{d}\lambda}{\lambda^{\frac12}}(\mathcal{R}_{1,\lambda}-\mathcal{R}_{0,\lambda})\Big),\tag{4.6}$$

as required. □

Remark 4.2. Combining the integral representation (4.5) with the equalities (4.3) and (4.4), one can represent the operator $\mathrm{g}(\mathcal{D}+V)-\mathrm{g}(\mathcal{D})$ as a sum of several Bochner integrals. The idea of the proof conducted in this section is that one can prove some of these integrals fall into the Schatten ideal $\mathcal{L}_{\frac{d}{2}}$ in the electric case and $\mathcal{L}_d$ in the magnetic case. We argue that if one can estimate the $\mathcal{L}_p$-valued function $f(\cdot)$, for $1\le p<\infty$, by

$$\big\|f(\lambda)\big\|_p=o\big((1+\lambda)^{-\frac12}\big),$$

then the Bochner integral

$$\int_0^\infty\frac{\mathrm{d}\lambda}{\lambda^{\frac12}}f(\lambda)$$

defines an operator belonging to $\mathcal{L}_p$.

In both the electric and magnetic cases, one of the integrals will admit (modulo the relevant Schatten ideal) a leading term, which we shall later prove (in Section 4.1.4 below) does not belong to the separable part of $\mathcal{L}_{\frac{d}{2},\infty}$ in the electric case, or the separable part of $\mathcal{L}_{d,\infty}$ in the magnetic case.

Next, we present the Cwikel estimates (see Section 2.5.2 above) in a form convenient for the proofs below. In the following, we let $\mathrm{F} = (f_{j,k})_{j,k=1}^{N_d} \in M_{N_d}\big(L_\infty(\mathbb{R}^d)\big)$ denote an $N_d \times N_d$ matrix of essentially bounded functions, and let M_{F} be the multiplication operator corresponding to F; that is, we let M_{F} be the bounded operator on $\mathbb{C}^{N_d} \otimes L_2(\mathbb{R}^d) \simeq L_2(\mathbb{R}^d)^{N_d}$ given by the expression

$$M_{\mathrm{F}} \coloneqq \sum_{j,k=1}^{d} P_{j,k} \otimes M_{f_{j,k}},$$

where, for $j, k = 1, \ldots, N_d$, the matrix $P_{j,k} \coloneqq (\delta_{m,j}\delta_{n,k})_{m,n=1}^{N_d} \in M_{N_d}(\mathbb{C})$, and where $\delta_{j,k}$ denotes the Kronecker delta. Additionally, for brevity, we let

$$\langle \mathbf{x} \rangle_\lambda \coloneqq \big(1 + \lambda + |\mathbf{x}|^2\big)^{\frac{1}{2}}, \quad \mathbf{x} \in \mathbb{R}^d, \, \lambda \geq 0.$$

Proposition 4.3. *Let $1 \leq p < \infty$ and $\lambda \geq 0$. Suppose $\alpha \in \mathbb{N}$ such that $\alpha > \frac{d}{p}$. We have the following estimates:*

(i) If $2 \leq p < \infty$ and $\mathrm{F} \in M_{N_d}\big((L_p \cap L_\infty)(\mathbb{R}^d)\big)$, then

$$M_{\mathrm{F}}\mathcal{R}_{0,\lambda}^{\alpha}, \; M_{\mathrm{F}}\big(\mathbb{I} \otimes \langle \nabla \rangle_\lambda^{-\alpha}\big) \in \mathcal{L}_p,$$

and

$$\|M_{\mathrm{F}}\mathcal{R}_{0,\lambda}^{\alpha}\|_p \leq \Big\|M_{\mathrm{F}}\big(\mathbb{I} \otimes \langle \nabla \rangle_\lambda^{-\alpha}\big)\Big\|_p \leq \mathrm{const} \cdot (1+\lambda)^{\frac{d}{2p} - \frac{\alpha}{2}} \cdot \max_{j,k} \|f_{j,k}\|_p.$$

(ii) If $1 \leq p < 2$ and $\mathrm{F} \in M_{N_d}\big((W_p^d \cap L_\infty)(\mathbb{R}^d)\big)$, then

$$M_{\mathrm{F}}\mathcal{R}_{0,\lambda}^{\alpha}, \; M_{\mathrm{F}}\big(\mathbb{I} \otimes \langle \nabla \rangle_\lambda^{-\alpha}\big) \in \mathcal{L}_p,$$

and

$$\|M_{\mathrm{F}}\mathcal{R}_{0,\lambda}^{\alpha}\|_p \leq \Big\|M_{\mathrm{F}}\big(\mathbb{I} \otimes \langle \nabla \rangle_\lambda^{-\alpha}\big)\Big\|_p \leq \mathrm{const} \cdot (1+\lambda)^{\frac{d}{4p} - \frac{\alpha}{4}} \cdot \max_{j,k} \|f_{j,k}\|_{W_p^d}.$$

Proof. Firstly, for every $\lambda \geq 0$, we note that since

$$|\mathcal{R}_{0,\lambda}| \overset{(4.2)}{=} \mathbb{I} \otimes (1 + \lambda - \Delta)^{-\frac{1}{2}} = \mathbb{I} \otimes \langle \nabla \rangle_\lambda^{-1}$$

it follows from the polar decomposition that if $M_{\mathrm{F}}\big(\mathbb{I} \otimes \langle \nabla \rangle_\lambda^{-\alpha}\big) \in \mathcal{L}_p$, then $M_{\mathrm{F}}\mathcal{R}_{0,\lambda}^{-\alpha} \in \mathcal{L}_p$, for all $1 \leq p < \infty$, and that

$$\begin{aligned}\|M_{\mathrm{F}}\mathcal{R}_{0,\lambda}^{-\alpha}\|_p \leq \Big\|M_{\mathrm{F}}\big(\mathbb{I} \otimes \langle \nabla \rangle_\lambda^{-\alpha}\big)\Big\|_p &\leq \sum_{j,k=1}^{N_d} \big\|P_{j,k} \otimes M_{f_{j,k}} \langle \nabla \rangle_\lambda^{-\alpha}\big\|_p \\ &\leq N_d^2 \cdot \max_{j,k} \big\|M_{f_{j,k}} \langle \nabla \rangle_\lambda^{-\alpha}\big\|_p.\end{aligned}$$

Part (i) then immediately follows from Theorem 2.45, since

$$\left\|\langle\cdot\rangle_\lambda^{-\alpha}\right\|_p = \mathrm{const}\cdot(1+\lambda)^{\frac{d}{2p}-\frac{\alpha}{2}}.$$

Part (ii) follows similarly from Theorem 2.50 and the fact that $W_p^d(\mathbb{R}^d)\subset \ell_p(L_2)(\mathbb{R}^d)$ (see Proposition 2.55 above), since

$$\left\|\langle\cdot\rangle_\lambda^{-\alpha}\right\|_{\ell_p(L_2)} \leq \mathrm{const}\cdot\left\|\langle\cdot\rangle^{\frac{\alpha p+d(1-p)}{2}}\langle\cdot\rangle_\lambda^{-\alpha}\right\|_2 \leq \mathrm{const}\cdot(1+\lambda)^{\frac{d}{4p}-\frac{\alpha}{4}},$$

where the second line follows from an argument similar to [79, p. 39]. □

Remark 4.4. We note that, since the operator $\mathbb{I}\otimes\langle\nabla\rangle_\lambda^{-\alpha}$, for $\alpha>0$, commutes with $A\otimes 1$, for any matrix $A\in M_{N_d}(\mathbb{C})$, it follows that, for any $\alpha,\beta>0$, we can write

$$\mathcal{R}_{0,\lambda}^{\alpha}(A\otimes 1)\mathcal{R}_{0,\lambda}^{\beta} = \big(\mathbb{I}\otimes\langle\nabla\rangle_\lambda^{-\alpha-\beta}\big)\cdot\big(\mathbb{I}\otimes\langle\nabla\rangle_\lambda^{\alpha}\big)\mathcal{R}_{0,\lambda}^{\alpha}(A\otimes 1)\big(\mathbb{I}\otimes\langle\nabla\rangle_\lambda^{\beta}\big)\mathcal{R}_{0,\lambda}^{\beta}.$$

In particular, via the functional calculus, the operator

$$\big(\mathbb{I}\otimes\langle\nabla\rangle_\lambda^{\alpha}\big)\mathcal{R}_{0,\lambda}^{\alpha} : \mathbb{C}^{N_d}\otimes L_2(\mathbb{R}^d)\to\mathbb{C}^{N_d}\otimes L_2(\mathbb{R}^d)$$

is bounded on $\mathbb{C}^{N_d}\otimes L_2(\mathbb{R}^d)$, for any $\alpha>0$. Hence, it follows that if $\mathcal{I}$ is a Banach ideal of $\mathcal{B}\big(\mathbb{C}^{N_d}\otimes L_2(\mathbb{R}^d)\big)$, then

$$V\mathcal{R}_{0,\lambda}^{\alpha}(A\otimes 1)\mathcal{R}_{0,\lambda}^{\beta}\in\mathcal{I} \qquad\Leftrightarrow\qquad V\big(\mathbb{I}\otimes\langle\nabla\rangle_\lambda^{-\alpha-\beta}\big)\in\mathcal{I},$$

and both operators share equivalent estimates in the norm $\|\cdot\|_{\mathcal{I}}$.

4.1.2 The decomposition for the electric case

In this section, we assume that the vector potential function $\mathbf{A}=0$, so that the perturbation of the Dirac operator is purely electric,

$$V=\mathbb{I}\otimes M_\phi,\quad \text{for real-valued } \phi\in L_\infty(\mathbb{R}^d), \tag{4.7}$$

and we seek a suitable decomposition. Recalling (4.4) and (4.6), we have the expression

$$\begin{aligned} &\mathrm{g}(\mathcal{D}+\mathbb{I}\otimes M_\phi)-\mathrm{g}(\mathcal{D})\\ &\overset{(4.4)}{\underset{(4.6)}{=}} \frac{1}{\pi}\,\mathfrak{Re}\Bigg(-\int_0^\infty\frac{\mathrm{d}\lambda}{\lambda^{\frac12}}\mathcal{R}_{1,\lambda}\big((\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\big)^3+\int_0^\infty\frac{\mathrm{d}\lambda}{\lambda^{\frac12}}\mathcal{R}_{0,\lambda}\big((\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\big)^2 \\ &\qquad\qquad -\int_0^\infty\frac{\mathrm{d}\lambda}{\lambda^{\frac12}}\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\Bigg). \end{aligned}\tag{4.8}$$

Lemma 4.5. *If $\phi\in(L_{\frac{3d}{2}}\cap L_\infty)(\mathbb{R}^d)$ is real-valued, then*

$$\int_0^\infty\frac{\mathrm{d}\lambda}{\lambda^{\frac12}}\mathcal{R}_{1,\lambda}\big((\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\big)^3\in\mathcal{L}_{\frac{d}{2}}.$$

Proof. By the definition of $\mathcal{R}_{1,\lambda}$ (see (4.1) above), we have that $\|\mathcal{R}_{1,\lambda}\|_\infty = (1+\lambda)^{-\frac{1}{2}}$. Moreover, by Proposition 4.3 (with $\alpha = 1$, $p = \frac{3d}{2}$), we have

$$\big\|(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\big\|_{\frac{3d}{2}} \leq \text{const}\cdot\|\phi\|_{\frac{3d}{2}}(1+\lambda)^{-\frac{1}{6}}.$$

Hence, by the Hölder inequality (see Theorem 2.19 above), we infer that

$$\begin{aligned}\Big\|\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\mathcal{R}_{1,\lambda}\big((\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\big)^3\Big\|_{\frac{d}{2}} &\leq \int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\big\|\mathcal{R}_{1,\lambda}\big((\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\big)^3\big\|_{\frac{d}{2}}\\ &\leq \int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\|\mathcal{R}_{1,\lambda}\|_\infty\big\|(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\big\|^3_{\frac{3d}{2}}\\ &\leq \text{const}\cdot\|\phi\|^3_{\frac{3d}{2}}\cdot\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}(1+\lambda)} < \infty,\end{aligned}$$

and so the result is proven. □

Before we obtain an $\mathcal{L}_{\frac{d}{2}}$-estimate for the second term on the right-hand side of (4.8), we state the following technical lemma, whose proof can be found in Appendix A.2 below.

Lemma 4.6. *We have*

$$\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\,\mathfrak{Re}(\mathcal{R}^3_{0,\lambda}) = -\frac{3\pi}{2}\mathcal{D}\langle\mathcal{D}\rangle^{-5}.$$

Lemma 4.7. *If $\phi \in (W^3_{\frac{d}{2}}\cap W^1_\infty)(\mathbb{R}^d)$ is real-valued, then*

$$\mathfrak{Re}\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\mathcal{R}_{0,\lambda}\big((\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\big)^2\Big) \in \mathcal{L}_{\frac{d}{2}}.$$

Proof. By Corollary 2.10, we have

$$\begin{aligned}&\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\\ &\qquad = \mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}^2_{0,\lambda}(\mathbb{I}\otimes M_\phi) - \mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}[\mathcal{R}_{0,\lambda},\mathbb{I}\otimes M_\phi]\\ &\qquad \overset{(2.7)}{=} \mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}^2_{0,\lambda}(\mathbb{I}\otimes M_\phi) + \sum_{k=1}^d \mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}^2_{0,\lambda}(\gamma_k\otimes M_{\partial_k\phi})\mathcal{R}_{0,\lambda}.\end{aligned}$$

Repeating this argument for the first term on the right-hand side of the above, we obtain that

$$\begin{aligned}&\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\\ &\qquad \overset{(2.7)}{=} (\mathbb{I}\otimes M_\phi)\mathcal{R}^3_{0,\lambda}(\mathbb{I}\otimes M_\phi) - \sum_{k=1}^d \mathcal{R}_{0,\lambda}(\gamma_k\otimes M_{\partial_k\phi})\mathcal{R}^3_{0,\lambda}(\mathbb{I}\otimes M_\phi)\\ &\qquad\quad + \sum_{k=1}^d \mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}^2_{0,\lambda}(\gamma_k\otimes M_{\partial_k\phi})\mathcal{R}_{0,\lambda}.\end{aligned} \tag{4.9}$$

By Remark 4.2, it suffices to show that each individual term on the right-hand side of (4.9) belongs to $\mathcal{L}_{\frac{d}{2}}$ and has $\mathcal{L}_{\frac{d}{2}}$-norm that is $o\big((1+\lambda)^{-\frac{1}{2}}\big)$.

Firstly, we treat the summands in the third term of (4.9). Fix $k = 1, \ldots, d$. Using the equality $\phi = |\phi|^{\frac{1}{2}} \cdot (\mathrm{sgn} \circ \phi) \cdot |\phi|^{\frac{1}{2}}$ together with the Hölder inequality (see Theorem 2.19 above), we write

$$\begin{aligned}\big\|\mathcal{R}_{0,\lambda}(\mathbb{I} \otimes M_\phi)\mathcal{R}_{0,\lambda}^2(\gamma_k \otimes M_{\partial_k\phi})\mathcal{R}_{0,\lambda}\big\|_{\frac{d}{2}} \\ \leq \big\|(\mathbb{I} \otimes M_{|\phi|^{\frac{1}{2}}})\mathcal{R}_{0,\lambda}\big\|_{\frac{3d}{2}}^2 \|\mathcal{R}_{0,\lambda}\|_\infty \big\|(\gamma_k \otimes M_{\partial_k\phi})\mathcal{R}_{0,\lambda}\big\|_{\frac{3d}{2}}.\end{aligned}$$

By Proposition 4.3 (with $\alpha = 1$, $p = \frac{3d}{2}$), we have

$$\big\|(\mathbb{I} \otimes M_{|\phi|^{\frac{1}{2}}})\mathcal{R}_{0,\lambda}\big\|_{\frac{3d}{2}} \leq \mathrm{const} \cdot \big\||\phi|^{\frac{1}{2}}\big\|_{\frac{3d}{2}}(1+\lambda)^{-\frac{1}{6}} \leq \mathrm{const} \cdot \|\phi\|_{\frac{3d}{4}}^{\frac{1}{2}}(1+\lambda)^{-\frac{1}{6}}.$$

and

$$\big\|(\gamma_k \otimes M_{\partial_k\phi})\mathcal{R}_{0,\lambda}\big\|_{\frac{3d}{2}} \leq \mathrm{const} \cdot \|\partial_k\phi\|_{\frac{3d}{2}}(1+\lambda)^{-\frac{1}{6}} \leq \mathrm{const} \cdot \|\phi\|_{W^1_{\frac{3d}{2}}}(1+\lambda)^{-\frac{1}{6}}. \tag{4.10}$$

Hence, we have the estimate

$$\begin{aligned}\big\|\mathcal{R}_{0,\lambda}(\mathbb{I} \otimes M_\phi)\mathcal{R}_{0,\lambda}^2(\gamma_k \otimes M_{\partial_k\phi})\mathcal{R}_{0,\lambda}\big\|_{\frac{d}{2}} &\leq \mathrm{const} \cdot \|\mathcal{R}_{0,\lambda}\|_\infty \|\phi\|_{\frac{3d}{4}} \|\phi\|_{W^1_{\frac{3d}{2}}}(1+\lambda)^{-\frac{1}{2}}, \\ &\leq \mathrm{const}_\phi \cdot (1+\lambda)^{-1},\end{aligned}$$

as required.

We may consider the $\mathcal{L}_{\frac{d}{2}}$-norm of the summand of the first series in (4.9) above in a similar fashion. The Hölder inequality (Theorem 2.19 above) gives the estimate

$$\big\|\mathcal{R}_{0,\lambda}(\gamma_k \otimes M_{\partial_k\phi})\mathcal{R}_{0,\lambda}^3(\mathbb{I} \otimes M_\phi)\big\|_{\frac{d}{2}} \leq \big\|(\gamma_k \otimes M_{\partial_k\phi})\mathcal{R}_{0,\lambda}\big\|_{\frac{3d}{2}} \big\|(\mathbb{I} \otimes M_\phi)\mathcal{R}_{0,\lambda}^3\big\|_{\frac{3d}{4}}.$$

If $d \geq 3$, then we may appeal to Proposition 4.3 (i) (with $\alpha = 3$, $p = \frac{3d}{4}$) to obtain the $\mathcal{L}_{\frac{3d}{4}}$-estimate

$$\big\|(\mathbb{I} \otimes M_\phi)\mathcal{R}_{0,\lambda}^3\big\|_{\frac{3d}{4}} \leq \mathrm{const} \cdot \|\phi\|_{\frac{3d}{4}}(1+\lambda)^{-\frac{5}{6}}.$$

In contrast, if $d = 2$, then Proposition 4.3 (ii) (with $\alpha = 3$, $p = \frac{3}{2}$) gives

$$\big\|(\mathbb{I} \otimes M_\phi)\mathcal{R}_{0,\lambda}^3\big\|_{\frac{3}{2}} \leq \mathrm{const} \cdot \|\phi\|_{W^2_{\frac{3}{2}}}(1+\lambda)^{-\frac{5}{12}}.$$

Hence, combining the above estimate with (4.10), we obtain

$$\big\|\mathcal{R}_{0,\lambda}(\gamma_k \otimes M_{\partial_k\phi})\mathcal{R}_{0,\lambda}^3\big\|_{\frac{d}{2}} \leq \begin{cases} \mathrm{const} \cdot \|\phi\|_{W^1_{\frac{3d}{2}}} \|\phi\|_{\frac{3d}{4}}(1+\lambda)^{-1}, & \text{if } d \geq 3, \\ \mathrm{const} \cdot \|\phi\|_{W^1_3} \|\phi\|_{W^2_{\frac{3}{2}}}(1+\lambda)^{-\frac{7}{12}}, & \text{if } d = 2. \end{cases}$$

Thus, it remains to show that

$$\Re\mathfrak{e}\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}(\mathbb{I} \otimes M_\phi)\mathcal{R}_{0,\lambda}^3(\mathbb{I} \otimes M_\phi)\Big) \in \mathcal{L}_{\frac{d}{2}}\big(\mathbb{C}^{N_d} \otimes L_2(\mathbb{R}^d)\big). \tag{4.11}$$

By Hille's theorem (see, e.g., [30, §II.2 Theorem 6]) and Lemma 4.6, we have that

$$\begin{aligned}\mathfrak{Re}\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac12}}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}^3(\mathbb{I}\otimes M_\phi)\Big) &= (\mathbb{I}\otimes M_\phi)\,\mathfrak{Re}\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac12}}\mathcal{R}_{0,\lambda}^3\Big)(\mathbb{I}\otimes M_\phi)\\ &= -\frac{3\pi}{2}(\mathbb{I}\otimes M_\phi)\mathcal{D}\langle\mathcal{D}\rangle^{-5}(\mathbb{I}\otimes M_\phi).\end{aligned}$$

By Proposition 4.3 (with $\alpha = 4$, $p = \frac{d}{2}$, $\lambda = 0$), we observe that

$$\big\|(\mathbb{I}\otimes M_\phi)\langle\mathcal{D}\rangle^{-4}\big\|_{\frac d2} \le \mathrm{const}\cdot\begin{cases}\|\phi\|_{\frac d2}, & \text{if } d\ge 4,\\ \|\phi\|_{W^3_{\frac32}}, & \text{if } d=3,\\ \|\phi\|_{W^2_1}, & \text{if } d=2.\end{cases}$$

Therefore, we conclude that

$$\begin{aligned}\Big\|\mathfrak{Re}\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac12}}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}^3(\mathbb{I}\otimes M_\phi)\Big)\Big\|_{\frac d2} &\le \frac{3\pi}{2}\big\|(\mathbb{I}\otimes M_\phi)\mathcal{D}\langle\mathcal{D}\rangle^{-5}(\mathbb{I}\otimes M_\phi)\big\|_{\frac d2}\\ &\le \frac{3\pi}{2}\big\|(\mathbb{I}\otimes M_\phi)\langle\mathcal{D}\rangle^{-4}\big\|_{\frac d2}\big\|\mathrm{g}(\mathcal{D})(\mathbb{I}\otimes M_\phi)\big\|_\infty < \infty.\ \square\end{aligned}$$

We arrive at the following intermediate lemma.

Lemma 4.8. *If $\phi \in (W^3_{\frac d2}\cap W^1_\infty)(\mathbb{R}^d)$ is real-valued, then*

$$\mathrm{g}(\mathcal{D}+\mathbb{I}\otimes M_\phi) - \mathrm{g}(\mathcal{D}) \in -\frac{1}{\pi}\,\mathfrak{Re}\Big(\int_0^\infty \mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\Big) + \mathcal{L}_{\frac d2}. \tag{4.12}$$

Proof. We infer the result by combining Lemmas 4.5 and 4.7 with the decomposition (4.8). □

Next, we treat the third term of (4.8). Since this is the last remaining term in the decomposition, we claim that this term is not in $\mathcal{L}_{\frac d2}$ (under stronger assumptions on ϕ). First, we shall need the following auxiliary lemma, whose proof can be found in Appendix A.2 below.

Lemma 4.9. (*i*) *Suppose $k \in \{1,\dots,d\}$. Then*

$$\begin{aligned}\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac12}}\big(\mathcal{R}_{0,\lambda}(\gamma_k\otimes 1)\mathcal{R}_{0,\lambda}^2 + \mathcal{R}_{0,\lambda}^*(\gamma_k\otimes 1)(\mathcal{R}_{0,\lambda}^*)^2\big)&\\ = \frac{\pi}{2}[\mathcal{D},\gamma_k\otimes 1]\langle\mathcal{D}\rangle^{-3} - \frac{3\pi}{2}\{\mathcal{D},\gamma_k\otimes 1\}\langle\mathcal{D}\rangle^{-5},&\end{aligned} \tag{4.13}$$

where $\{\cdot,\cdot\}$ denotes the anticommutator.

(*ii*) *We have*

$$\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac12}}\,\mathfrak{Re}(\mathcal{R}_{0,\lambda}^2) = -2\pi\langle\mathcal{D}\rangle^{-3}.$$

We define the following operator for brevity. For $\phi \in W^1_\infty(\mathbb{R}^d)$, let

$$\Phi_{j,k} := (M_{\partial_j\phi}\partial_k - M_{\partial_k\phi}\partial_j)\langle\nabla\rangle^{-3} \in \mathcal{B}\big(L_2(\mathbb{R}^d)\big), \quad j,k = 1,\dots,d. \tag{4.14}$$

Lemma 4.10. *If $\phi \in (W^5_{\frac{d}{2}} \cap W^5_\infty)(\mathbb{R}^d)$ is real-valued, then*

$$\mathfrak{Re}\Big(\int_0^\infty \mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\Big) \in \frac{\pi}{2}\sum_{j>k}\gamma_j\gamma_k\otimes\Phi_{j,k} + \mathcal{L}_{\frac{d}{2}}.$$

Proof. The general strategy we employ is to shift the $\mathcal{R}_{0,\lambda}$ terms towards the right using Corollary 2.10, and then follow up with Cwikel estimates on the leftover terms. That is, we consider

$$\begin{aligned}\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda} &\overset{(2.7)}{=} (\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}^2 - \sum_{k=1}^d \big(\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_{\partial_k\phi})\big)(\gamma_k\otimes 1)\mathcal{R}_{0,\lambda}^2\\ &\overset{(2.7)}{=} (\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}^2 - \sum_{k=1}^d(\mathbb{I}\otimes M_{\partial_k\phi})\mathcal{R}_{0,\lambda}(\gamma_k\otimes 1)\mathcal{R}_{0,\lambda}^2\\ &\quad + \sum_{j,k=1}^d \mathcal{R}_{0,\lambda}(\gamma_j\otimes M_{\partial_j\partial_k\phi})\mathcal{R}_{0,\lambda}(\gamma_k\otimes 1)\mathcal{R}_{0,\lambda}^2.\end{aligned} \tag{4.15}$$

We briefly focus on the summand of the third term of this decomposition, and fix $j,k = 1,\dots,d$. By Remark 4.4 and the Hölder inequality (see Theorem 2.19 above), we have

$$\begin{aligned}\big\|\mathcal{R}_{0,\lambda}(\gamma_j\otimes M_{\partial_j\partial_k\phi})\mathcal{R}_{0,\lambda}(\gamma_k\otimes 1)\mathcal{R}_{0,\lambda}^2\big\|_{\frac{d}{2}} &\overset{(4.2)}{\leq} \big\|\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_{\partial_j\partial_k\phi})\langle\mathcal{D}\rangle_\lambda^{-3}\big\|_{\frac{d}{2}}\\ &\leq \|\mathcal{R}_{0,\lambda}\|_\infty\big\|(\mathbb{I}\otimes M_{\partial_j\partial_k\phi})\langle\mathcal{D}\rangle_\lambda^{-3}\big\|_{\frac{d}{2}}.\end{aligned} \tag{4.16}$$

If $d \geq 4$, then we may appeal to Proposition 4.3 (i) (with $\alpha = 3$, $p = \frac{d}{2}$) to obtain

$$\big\|(\mathbb{I}\otimes M_{\partial_j\partial_k\phi})\langle\mathcal{D}\rangle_\lambda^{-3}\big\|_{\frac{d}{2}} \leq \mathrm{const}\cdot\|\partial_j\partial_k\phi\|_{\frac{d}{2}}(1+\lambda)^{-\frac{1}{2}} \leq \mathrm{const}\cdot\|\phi\|_{W^2_{\frac{d}{2}}}(1+\lambda)^{-\frac{1}{2}}.$$

If $d = 2,3$, then Proposition 4.3 (ii) (with $\alpha = 3$, $p = \frac{d}{2}$) yields

$$\big\|(\mathbb{I}\otimes M_{\partial_j\partial_k\phi})\langle\mathcal{D}\rangle_\lambda^{-3}\big\|_{\frac{d}{2}} \leq \mathrm{const}\cdot\|\partial_j\partial_k\phi\|_{W^d_{\frac{d}{2}}}(1+\lambda)^{-\frac{1}{4}} \leq \mathrm{const}\cdot\|\phi\|_{W^{d+2}_{\frac{d}{2}}}(1+\lambda)^{-\frac{1}{4}}.$$

Therefore, since $\|\mathcal{R}_{0,\lambda}\|_\infty = (1+\lambda)^{-\frac{1}{2}}$, the left-hand side of (4.16) above may be estimated by

$$\big\|\mathcal{R}_{0,\lambda}(\gamma_j\otimes M_{\partial_j\partial_k\phi})\mathcal{R}_{0,\lambda}(\gamma_k\otimes 1)\mathcal{R}_{0,\lambda}^2\big\|_{\frac{d}{2}} = \begin{cases}\mathrm{const}\cdot\|\phi\|_{W^2_{\frac{d}{2}}}(1+\lambda)^{-1}, & \text{if } d\geq 4,\\ \mathrm{const}\cdot\|\phi\|_{W^5_{\frac{3}{2}}}(1+\lambda)^{-\frac{3}{4}}, & \text{if } d = 3,\\ \mathrm{const}\cdot\|\phi\|_{W^4_1}(1+\lambda)^{-\frac{3}{4}}, & \text{if } d = 2.\end{cases} \tag{4.17}$$

Hence, by Remark 4.2, the Bochner integral of the third term in (4.15) belongs to $\mathcal{L}_{\frac{d}{2}}$.

We treat the operator $(\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda})^*$ similarly. Since ϕ is real-valued, we have that $M^*_{\partial_k\phi} = -M_{\partial_k\phi}$ and $M^*_{\partial_j\partial_k\phi} = M_{\partial_j\partial_k\phi}$. We may appeal to Corollary 2.10 to shift $\mathbb{I}\otimes M_\phi$ to the right instead of the left before taking the adjoint. Hence, we observe that

$$\begin{aligned}\big(\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\big)^* = (\mathbb{I}\otimes M_\phi)(\mathcal{R}^*_{0,\lambda})^2 - \sum_{k=1}^d (\mathbb{I}\otimes M_{\partial_k\phi})\mathcal{R}^*_{0,\lambda}(\gamma_k\otimes 1)(\mathcal{D}^*_{0,\lambda})^2 \\ + \sum_{j,k=1}^d \mathcal{R}^*_{0,\lambda}(\gamma_j\otimes M_{\partial_j\partial_k\phi})\mathcal{R}^*_{0,\lambda}(\gamma_k\otimes 1)(\mathcal{R}^*_{0,\lambda})^2,\end{aligned} \tag{4.18}$$

and, by a similar argument to that of (4.17), we arrive at

$$\big\|\mathcal{R}^*_{0,\lambda}(\gamma_j\otimes M_{\partial_j\partial_k\phi})\mathcal{R}^*_{0,\lambda}(\gamma_k\otimes 1)(\mathcal{R}^*_{0,\lambda})^2\big\|_{\frac{d}{2}} = \begin{cases}\mathrm{const}\cdot\|\phi\|_{W^2_{\frac{d}{2}}}(1+\lambda)^{-1}, & \text{if } d\geq 4,\\ \mathrm{const}\cdot\|\phi\|_{W^5_{\frac{3}{2}}}(1+\lambda)^{-\frac{3}{4}}, & \text{if } d=3,\\ \mathrm{const}\cdot\|\phi\|_{W^3_1}(1+\lambda)^{-\frac{3}{4}}, & \text{if } d=2.\end{cases} \tag{4.19}$$

Hence, combining Lemma 4.9 (i) with (4.15), (4.17), (4.18) and (4.19), one obtains the expression

$$\begin{aligned}\mathfrak{Re}\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\Big) &= \frac{1}{2}\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\Big(\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda} + \big(\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\big)^*\Big)\\ &\in \frac{1}{2}\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\big((\mathbb{I}\otimes M_\phi)\mathcal{R}^2_{0,\lambda} + (\mathbb{I}\otimes M_\phi)(\mathcal{R}^*_{0,\lambda})^2\big)\\ &\quad - \frac{1}{2}\sum_{k=1}^d(\mathbb{I}\otimes M_{\partial_k\phi})\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\big(\mathcal{R}_{0,\lambda}(\gamma_k\otimes 1)\mathcal{R}^2_{0,\lambda} + \mathcal{R}^*_{0,\lambda}(\gamma_k\otimes 1)(\mathcal{R}^*_{0,\lambda})^2\big) + \mathcal{L}_{\frac{d}{2}}\\ &\overset{(4.13)}{=} \frac{\mathbb{I}\otimes M_\phi}{2}\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\,\mathfrak{Re}(\mathcal{R}^2_{0,\lambda}) - \frac{\pi}{4}\sum_{k=1}^d(\mathbb{I}\otimes M_{\partial_k\phi})[\mathcal{D},\gamma_k\otimes 1]\langle\mathcal{D}\rangle^{-3}\\ &\quad - \frac{3\pi}{4}\sum_{k=1}^d(\mathbb{I}\otimes M_{\partial_k\phi})\{\mathcal{D},\gamma_k\otimes 1\}\langle\mathcal{D}\rangle^{-5} + \mathcal{L}_{\frac{d}{2}}.\end{aligned} \tag{4.20}$$

Firstly, by Proposition 4.3 (with $\lambda = 0$, $p = \frac{d}{2}$, $\alpha = 4$), we observe that

$$\begin{aligned}\Big\|(\mathbb{I}\otimes M_{\partial_k\phi})\{\mathcal{D},\gamma_k\otimes 1\}\langle\mathcal{D}\rangle^{-5}\Big\|_{\frac{d}{2}} &\leq 2\big\|(\mathbb{I}\otimes M_{\partial_k\phi})\langle\mathcal{D}\rangle^{-4}\big\|_{\frac{d}{2}}\\ &\leq \begin{cases}\mathrm{const}\cdot\|\phi\|_{W^1_{\frac{d}{2}}}, & \text{if } d\geq 4,\\ \mathrm{const}\cdot\|\phi\|_{W^4_{\frac{3}{2}}}, & \text{if } d=3,\\ \mathrm{const}\cdot\|\phi\|_{W^3_1}, & \text{if } d=2,\end{cases}\end{aligned}$$

so the third term of (4.20) lies in $\mathcal{L}_{\frac{d}{2}}$.

Next, consider the first term of (4.20). By Lemma 4.9 (*ii*), we have that

$$\frac{\mathbb{I}\otimes M_\phi}{2}\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\,\Re\mathfrak{e}(\mathcal{R}_{0,\lambda}^2) = -\pi(\mathbb{I}\otimes M_f)\langle\mathcal{D}\rangle^{-3}.$$

Hence, by Proposition 4.3 (with $\lambda = 0$, $p = \frac{d}{2}$, $\alpha = 3$), we observe that

$$\begin{aligned}\Big\|\frac{\mathbb{I}\otimes M_\phi}{2}\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\,\Re\mathfrak{e}(\mathcal{R}_{0,\lambda}^2)\Big\|_{\frac{d}{2}} &= \pi\big\|(\mathbb{I}\otimes M_\phi)\langle\mathcal{D}\rangle^{-3}\big\|_{\frac{d}{2}}\\ &\le \begin{cases}\text{const}\cdot\|\phi\|_{\frac{d}{2}}, & \text{if } d\ge 4,\\ \text{const}\cdot\|\phi\|_{W^3_{\frac{3}{2}}}, & \text{if } d=3,\\ \text{const}\cdot\|\phi\|_{W^2_1}, & \text{if } d=2,\end{cases}\end{aligned}$$

so we additionally have that the first term of (4.20) is in $\mathcal{L}_{\frac{d}{2}}$.

Thus, only the second term of (4.20) remains to be treated; indeed, we have that

$$\begin{aligned}\Re\mathfrak{e}\Big(\int_0^\infty \mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\Big) &\overset{(4.20)}{=} \frac{\pi}{4}\sum_{k=1}^d(\mathbb{I}\otimes M_{\partial_k\phi})[\gamma_k\otimes 1,\mathcal{D}]\langle\mathcal{D}\rangle^{-3} + \mathcal{L}_{\frac{d}{2}}\\ &= \frac{\pi}{4}\sum_{k=1}^d\sum_{j=1}^d\big((\gamma_k\gamma_j-\gamma_j\gamma_k)\otimes M_{\partial_k\phi}\partial_j\big)\langle\mathcal{D}\rangle^{-3}+\mathcal{L}_{\frac{d}{2}}\\ &= \frac{\pi}{2}\sum_{j>k}\big(\gamma_j\gamma_k\otimes(M_{\partial_j\phi}\partial_k - M_{\partial_k\phi}\partial_j)\big)\langle\mathcal{D}\rangle^{-3}+\mathcal{L}_{\frac{d}{2}}.\end{aligned}$$

Referring to the definition of $\Phi_{j,k}$ (see (4.14)), we conclude the proof. □

Proposition 4.11. *If $\phi \in (W^5_{\frac{d}{2}}\cap W^5_\infty)(\mathbb{R}^d)$ is real-valued, then*

$$\mathrm{g}(\mathcal{D}+\mathbb{I}\otimes M_\phi) - \mathrm{g}(\mathcal{D}) \in -\frac{1}{2}\sum_{j>k}\gamma_j\gamma_k\otimes\Phi_{j,k} + \mathcal{L}_{\frac{d}{2}}.$$

Proof. One obtains the claim by combining Lemmas 4.8 and 4.10 above. □

Remark 4.12. Suppose we have real-valued $\phi \in (W^5_{\frac{d}{2}}\cap W^5_\infty)(\mathbb{R}^d)$, as above. Proposition 4.3 (with $p = d$, $\alpha = 2$) implies that $M_{\partial_j\phi}\langle\nabla\rangle^{-2}\in\mathcal{L}_d$ for every $j = 1,\dots,d$. Hence, $\Phi_{j,k}\in\mathcal{L}_d$, for every $j,k = 1,\dots,d$, and therefore,

$$\Re\mathfrak{e}\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\Big) \in \frac{\pi}{2}\sum_{j>k}\gamma_j\gamma_k\otimes\Phi_{j,k}+\mathcal{L}_{\frac{d}{2}}\subseteq\mathcal{L}_d.$$

4.1.3 The decomposition for the magnetic case

In this section, we obtain a similar decomposition as that of Proposition 4.11 in the general electromagnetic setting—with the perturbation

$$V = \mathbb{I}\otimes M_\phi - \sum_{j=1}^d\gamma_j\otimes M_{a_j}$$

under the assumption that $\mathbf{A} = (a_1,\dots,a_d)\neq 0$.

Lemma 4.13. *If $\phi, a_1, \ldots, a_d \in (L_{2d} \cap L_\infty)(\mathbb{R}^d)$, then*

$$\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) \in -\frac{1}{\pi}\,\mathfrak{Re}\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\mathcal{R}_{0,\lambda}V\mathcal{R}_{0,\lambda}\Big) + \mathcal{L}_d. \tag{4.21}$$

Proof. By a similar argument to (4.8), we have by (4.3) and (4.6) that

$$\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) = \frac{1}{\pi}\,\mathfrak{Re}\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\mathcal{R}_{1,\lambda}(V\mathcal{R}_{0,\lambda})^2 - \int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\mathcal{R}_{0,\lambda}V\mathcal{R}_{0,\lambda}\Big).$$

By the definition of $\mathcal{R}_{1,\lambda}$ (see (4.1)), we have that $\|\mathcal{R}_{1,\lambda}\|_\infty = (1+\lambda)^{-\frac{1}{2}}$. Moreover, by Proposition 4.3 (with $p = 2d$, $\alpha = 1$), we obtain the estimate

$$\|V\mathcal{R}_{0,\lambda}\|_{2d} \le \mathrm{const}\cdot\Big(\|\phi\|_{2d} + \sum_{j=1}^d \|a_j\|_{2d}\Big)(1+\lambda)^{-\frac{1}{4}}.$$

Hence, by Hölder's inequality (see Theorem 2.19 above), we obtain

$$\begin{aligned}\Big\|\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\mathcal{R}_{1,\lambda}(V\mathcal{R}_{0,\lambda})^2\Big\|_d &\le \int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\big\|\mathcal{R}_{1,\lambda}(V\mathcal{R}_{0,\lambda})^2\big\|_d \\ &\le \int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\|\mathcal{R}_{1,\lambda}\|_\infty\|V\mathcal{R}_{0,\lambda}\|_{2d}^2 \\ &= \mathrm{const}\cdot\Big(\|\phi\|_{2d} + \sum_{j=1}^d\|a_j\|_{2d}\Big)\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}(1+\lambda)}.\end{aligned}$$ □

We claim that the remaining term on the right-hand side of (4.21),

$$-\frac{1}{\pi}\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\,\mathfrak{Re}\left(\mathcal{R}_{0,\lambda}V\mathcal{R}_{0,\lambda}\right) \notin \mathcal{L}_d.$$

Before we treat this term, we need the following auxiliary lemma, whose proof can be found in Appendix A.2. For brevity, we let $\mathcal{D}_j$ denote (unbounded) operator with domain $\mathbb{C}^{N_d}\otimes W_2^1(\mathbb{R}^d)$ defined by

$$\mathcal{D}_j := \mathcal{D} - 2\gamma_j\otimes\partial_j, \qquad j\in\{1,\ldots,d\}. \tag{4.22}$$

By construction, for every $j = 1,\ldots,d$, the anticommutativity of the gamma matrices yields the identity

$$\mathcal{D}(\gamma_j\otimes 1) \overset{(2.4)}{=} \sum_{k=1}^d \gamma_k\gamma_j\otimes\partial_k = 2\mathbb{I}\otimes\partial_j - \sum_{k=1}^d\gamma_j\gamma_k\otimes\partial_k \overset{(4.22)}{=} -(\gamma_j\otimes 1)\mathcal{D}_j. \tag{4.23}$$

Lemma 4.14. *If $j = 1,\ldots,d$, then*

$$\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\,\mathfrak{Re}\left(\mathcal{R}_{0,\lambda}(\gamma_j\otimes 1)\mathcal{R}_{0,\lambda}\right) = -\frac{\pi}{2}(\gamma_j\otimes 1)(\mathcal{D}^2 + \mathcal{D}_j\mathcal{D})\langle\mathcal{D}\rangle^{-3} - \pi(\gamma_j\otimes 1)\langle\mathcal{D}\rangle^{-3}. \tag{4.24}$$

Since $\partial_j\partial_k\langle\nabla\rangle^{-2}$, for $j,k = 1,\ldots d$, are bounded operators on $L_2(\mathbb{R}^d)$, for $a_j\in L_\infty(\mathbb{R}^d)$, $j = 1,\ldots,d$, one may define a bounded operator on $\mathbb{C}^{N_d}\otimes L_2(\mathbb{R}^d)$ by

$$\Psi_j := \sum_{k=1}^d (M_{a_k}\partial_j\partial_k - M_{a_j}\partial_k^2)\langle\nabla\rangle^{-3}, \quad \text{for } j = 1,\ldots,d, \tag{4.25}$$

Proposition 4.15. *If* $\phi \in (W^5_{\frac{d}{2}} \cap W^5_\infty)(\mathbb{R}^d)$ *and* $\mathbf{A} \in (W^1_d \cap W^1_\infty)(\mathbb{R}^d)^d$, *then*

$$\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) \in -\sum_{j=1}^d \gamma_j \otimes \Psi_j + \mathcal{L}_d.$$

Proof. By Lemma 4.13, we have that

$$\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) \in -\frac{1}{\pi}\,\mathfrak{Re}\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac12}}\mathcal{R}_{0,\lambda}V\mathcal{R}_{0,\lambda}\Big) + \mathcal{L}_d.$$

However, by Remark 4.12, we already have that

$$\mathfrak{Re}\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac12}}\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_\phi)\mathcal{R}_{0,\lambda}\Big) \in \mathcal{L}_d.$$

Hence, without loss of generality, we may assume that

$$V = -\sum_{j=1}^d \gamma_j \otimes M_{a_j}.$$

By Corollary 2.10, we have that

$$\begin{aligned}\mathcal{R}_{0,\lambda}V\mathcal{R}_{0,\lambda} &= -\sum_{j=1}^d \mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_{a_j})(\gamma_j\otimes 1)\mathcal{R}_{0,\lambda}\\ &\overset{(2.7)}{=} -\sum_{j=1}^d (\mathbb{I}\otimes M_{a_j})\mathcal{R}_{0,\lambda}(\gamma_j\otimes 1)\mathcal{R}_{0,\lambda} - \sum_{j,k=1}^d \mathcal{R}_{0,\lambda}(\gamma_k\otimes M_{\partial_k a_j})\mathcal{R}_{0,\lambda}(\gamma_j\otimes 1)\mathcal{R}_{0,\lambda}.\end{aligned} \tag{4.26}$$

Similarly, for $(\mathcal{R}_{0,\lambda}V\mathcal{R}_{0,\lambda})^*$, we obtain the identity

$$(\mathcal{R}_{0,\lambda}V\mathcal{R}_{0,\lambda})^* = -\sum_{j=1}^d (\mathbb{I}\otimes M_{a_j})\mathcal{R}^*_{0,\lambda}(\gamma_j\otimes 1)\mathcal{R}^*_{0,\lambda} - \sum_{j,k=1}^d \mathcal{R}^*_{0,\lambda}(\gamma_k\otimes M_{\partial_k a_j})\mathcal{R}^*_{0,\lambda}(\gamma_j\otimes 1)\mathcal{R}^*_{0,\lambda} \tag{4.27}$$

Consider the second term of (4.26). Fixing $j,k = 1,\dots,d$, one may appeal to the Hölder inequality (see Theorem 2.19 above) and Remark 4.4 to get

$$\begin{aligned}\big\|\mathcal{R}_{0,\lambda}(\gamma_k\otimes M_{\partial_k a_j})\mathcal{R}_{0,\lambda}(\gamma_j\otimes 1)\mathcal{R}_{0,\lambda}\big\|_d &\le \big\|\mathcal{R}_{0,\lambda}(\mathbb{I}\otimes M_{\partial_k a_j})\langle\mathcal{D}\rangle_\lambda^{-2}\big\|_d\\ &\le \|\mathcal{R}_{0,\lambda}\|_\infty \big\|\mathbb{I}\otimes M_{\partial_k a_j}\langle\nabla\rangle_\lambda^{-2}\big\|_d.\end{aligned}$$

By Proposition 4.3 (with $p = d$, $\alpha = 2$), we have that

$$\big\|\mathbb{I}\otimes M_{\partial_k a_j}\langle\nabla\rangle_\lambda^{-2}\big\|_d \le \mathrm{const}\cdot\|\partial_k a_j\|_d(1+\lambda)^{-\frac12} \le \mathrm{const}\cdot\|a_j\|_{W^1_d}(1+\lambda)^{-\frac12}.$$

Therefore, since $\|\mathcal{R}_{0,\lambda}\|_\infty \le (1+\lambda)^{-\frac12}$, we observe that

$$\big\|\mathcal{R}_{0,\lambda}(\gamma_k\otimes M_{\partial_k a_j})\mathcal{R}_{0,\lambda}(\gamma_j\otimes 1)\mathcal{R}_{0,\lambda}\big\|_d = \mathrm{const}_{a_j}\cdot(1+\lambda)^{-1}.$$

Hence, by Remark 4.2, the Bochner integral of the second term of (4.26) belongs to $\mathcal{L}_d$. By a similar argument, we also observe that the Bochner integral of the second term of (4.27) belongs to $\mathcal{L}_d$.

It remains to consider the first terms of both (4.26) and (4.27). By Lemma 4.14, we obtain

$$\begin{aligned}\mathfrak{Re}\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\mathcal{R}_{0,\lambda}V\mathcal{R}_{0,\lambda}\Big) &\in -\sum_{j=1}^d \int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}(\mathbb{I}\otimes M_{a_j})\,\mathfrak{Re}\left(\mathcal{R}_{0,\lambda}(\gamma_j\otimes 1)\mathcal{R}_{0,\lambda}\right)+\mathcal{L}_d\\ &\overset{(4.24)}{=} \frac{\pi}{2}\sum_{j=1}^d(\gamma_j\otimes M_{a_j})(\mathcal{D}^2+\mathcal{D}_j\mathcal{D})\langle\mathcal{D}\rangle^{-3}+\pi\sum_{j=1}^d(\gamma_j\otimes M_{a_j})\langle\mathcal{D}\rangle^{-3}+\mathcal{L}_d.\end{aligned}$$

However, for each $j=1,\dots,d$, Proposition 4.3 (with $\lambda=0$, $p=d$, $\alpha=3$) implies that $(\gamma_j\otimes M_{a_j})\langle\mathcal{D}\rangle^{-3}\in\mathcal{L}_d$, so we have that

$$\mathfrak{Re}\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\mathcal{R}_{0,\lambda}V\mathcal{R}_{0,\lambda}\Big) = \frac{\pi}{2}\sum_{j=1}^d(\gamma_j\otimes M_{a_j})(\mathcal{D}^2+\mathcal{D}_j\mathcal{D})\langle\mathcal{D}\rangle^{-3}+\mathcal{L}_d.$$

By the definition of $\mathcal{D}_j$ (see (4.22) above), we observe that

$$\mathcal{D}^2+\mathcal{D}_j\mathcal{D}=2\mathcal{D}^2-2(\gamma_j\otimes\partial_j)\mathcal{D}.$$

Hence, taking the sum and appealing to the definition of $\mathcal{D}$, we have that

$$\begin{aligned}\frac{1}{2}\sum_{j=1}^d(\gamma_j\otimes M_{a_j})(\mathcal{D}^2+\mathcal{D}_j\mathcal{D}) &= \sum_{j=1}^d(\gamma_j\otimes M_{a_j})\big(\mathcal{D}^2-(\gamma_j\otimes\partial_j)\mathcal{D}\big)\\ &\overset{(2.4)}{=}\sum_{j,k=1}^d \gamma_j\otimes M_{a_j}\partial_k^2-\sum_{j,k=1}^d\gamma_k\otimes M_{a_j}\partial_j\partial_k\\ &=\sum_{j,k=1}^d\gamma_j\otimes(M_{a_j}\partial_k^2-M_{a_k}\partial_j\partial_k),\end{aligned}$$

on the domain $\mathrm{dom}(\mathcal{D}^2)=\mathbb{C}^{N_d}\otimes W_2^2(\mathbb{R}^d)$. Therefore, by Lemma 4.13, we have

$$\begin{aligned}\mathrm{g}(\mathcal{D}+V)-\mathrm{g}(\mathcal{D}) &\overset{(4.21)}{\in} -\frac{1}{\pi}\,\mathfrak{Re}\Big(\int_0^\infty\frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\mathcal{R}_{0,\lambda}V\mathcal{R}_{0,\lambda}\Big)+\mathcal{L}_d\\ &=\sum_{j,k=1}^d\gamma_j\otimes(M_{a_j}\partial_k^2-M_{a_k}\partial_j\partial_k)\langle\mathcal{D}\rangle^{-3}+\mathcal{L}_d,\end{aligned}$$

which, by construction of Ψ_j (see (4.25) above), concludes the proof. □

4.1.4 Optimal estimates for $\mathrm{g}(\mathcal{D}+V)-\mathrm{g}(\mathcal{D})$

In the first result of this section we use Propositions 4.11 and 4.15 to show that the operator $\mathrm{g}(\mathcal{D}+V)-\mathrm{g}(\mathcal{D})$ belongs to the weak Schatten ideal, which proves one of the assertions of Theorem 1.9.

Theorem 4.16. *Suppose* $\phi \in (W^5_{\frac{d}{2}} \cap W^5_\infty)(\mathbb{R}^d)$ *and* $\mathbf{A} \in (W^2_{\frac{d}{2}} \cap W^2_\infty)(\mathbb{R}^d)^d$.

(*i*) *If* $\mathbf{A} = 0$, *then* $\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) \in \mathcal{L}_{\frac{d}{2},\infty}$.

(*ii*) *If* $\mathbf{A} \neq 0$, *then* $\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) \in \mathcal{L}_{d,\infty}$.

Proof. Observe that the conditions on ϕ and $a_1, \dots, a_d$ below guarantee that assumptions of both Propositions 4.11 and 4.15 are satisfied. Therefore, the representations of Proposition 4.11 and 4.15 are both valid.

(i). Suppose $\mathbf{A} = 0$. By Proposition 4.11, we have that

$$\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) \in \frac{1}{2}\sum_{j>k} \gamma_j\gamma_k \otimes \Phi_{j,k} + \mathcal{L}_{\frac{d}{2}},$$

so it suffices to show that

$$\Phi_{j,k} = \frac{1}{2}(M_{\partial_j\phi}\partial_k - M_{\partial_k\phi}\partial_j)(1-\Delta)^{-\frac{3}{2}} \in \mathcal{L}_{\frac{d}{2},\infty},$$

for all $j,k = 1,\dots,d$. Since $\partial_j\langle\nabla\rangle^{-1}$, $\partial_k\langle\nabla\rangle^{-1} \in \mathcal{B}\big(L_2(\mathbb{R}^d)\big)$, it suffices to show that $M_{\partial_j\phi}\langle\nabla\rangle^{-2}$ belongs to $\mathcal{L}_{\frac{d}{2},\infty}$ for every $j = 1,\dots,d$. To show this, there are three distinct cases to consider.

Case 1. Suppose $d \geq 5$. Since $\partial_j\phi \in L_{\frac{d}{2}}(\mathbb{R}^d)$ by assumption, for every $j = 1,\dots,d$, Proposition 2.56 (i) (with $p = \frac{d}{2}$, $\delta = 2$) implies that $M_{\partial_j\phi}\langle\nabla\rangle^{-2} \in \mathcal{L}_{\frac{d}{2},\infty}$, as required.

Case 2. Suppose $d = 2,3$. Since $\partial_j\phi \in W^d_{\frac{d}{2}}(\mathbb{R}^d)$ by assumption, for every $j = 1,\dots,d$, Proposition 2.56 (ii) (with $p = \frac{d}{2}$, $\delta = 2$) implies that $M_{\partial_j\phi}\langle\nabla\rangle^{-2} \in \mathcal{L}_{\frac{d}{2},\infty}$, as required.

Case 3. Suppose $d = 4$. Since $\partial_j\phi \in W^2_1(\mathbb{R}^4)$ by assumption, for every $j = 1,\dots,4$. Proposition 2.56 (iii) (with $\delta = 1$) implies that $M_{\partial_j\phi}\langle\nabla\rangle^{-2} \in \mathcal{L}_{2,\infty}$, and we are done.

(ii). Suppose $\mathbf{A} \neq 0$. By Proposition 4.15, we have that

$$\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) \in \sum_{j=1}^{d} \gamma_j \otimes \Psi_j + \mathcal{L}_d.$$

so it suffices to show that

$$\Psi_j = \sum_{k=1}^{d}(M_{a_k}\partial_j\partial_k - M_{a_j}\partial_k^2)\langle\nabla\rangle^{-3} \in \mathcal{L}_{d,\infty},$$

for every $j = 1,\dots,d$. Since $\partial_k^2\langle\nabla\rangle^{-2}$, $\partial_j\partial_k\langle\nabla\rangle^{-2} \in \mathcal{B}\big(L_2(\mathbb{R}^d)\big)$, it suffices to show that $M_{a_j}\langle\nabla\rangle^{-1} \in \mathcal{L}_{d,\infty}$ for all $j = 1,\dots,d$. To show this, there are two distinct cases to consider.

Case 1. Suppose $d \geq 3$. The assumption that $a_j \in L_d(\mathbb{R}^d)$, for every $j = 1,\dots,d$ together with Proposition 2.56 (i) (with $p = d$, $\delta = 1$) implies that $M_{a_j}\langle\nabla\rangle^{-1} \in \mathcal{L}_{d,\infty}$, as required.

CASE 2. Suppose $d = 2$. Since $a_j \in W_2^2(\mathbb{R}^2)$ by assumption, for each $j = 1, 2$, Proposition 2.56 (*iii*) (with $\delta = \frac{1}{2}$) implies that $M_{a_j}\langle\nabla\rangle^{-1} \in \mathcal{L}_{2,\infty}$, which completes the proof. $\square$

Theorem 4.17. *Suppose* $\phi \in (W^5_{\frac{d}{2}} \cap W^5_\infty)(\mathbb{R}^d)$ *and* $\mathbf{A} \in (W^2_{\frac{d}{2}} \cap W^2_\infty)(\mathbb{R}^d)^d$.

(*i*) *If* $\mathbf{A} = 0$ *and* $\phi \neq 0$, *then* $\mathrm{g}(\mathcal{D} + V) - \mathrm{g}(\mathcal{D}) \notin (\mathcal{L}_{\frac{d}{2},\infty})_0$.

(*ii*) *If* $\mathbf{A} \neq 0$, *then* $\mathrm{g}(\mathcal{D} + V) - \mathrm{g}(\mathcal{D}) \notin (\mathcal{L}_{d,\infty})_0$.

Proof. (*i*). Suppose $\mathbf{A} = 0$, but $\phi \neq 0$. Assume to the contrary of the claim that $\mathrm{g}(\mathcal{D} + \mathbb{I} \otimes M_\phi) - \mathrm{g}(\mathcal{D}) \in (\mathcal{L}_{\frac{d}{2},\infty})_0$. By this assumption, and by Proposition 4.11, we have that

$$\sum_{j>k} \gamma_j\gamma_k \otimes \Phi_{j,k} \in (\mathcal{L}_{\frac{d}{2},\infty})_0.$$

Hence, by Lemma 2.12 (*ii*), we have that

$$\Phi_{j,k} = (M_{\partial_j\phi}\partial_k - M_{\partial_k\phi}\partial_j)\langle\nabla\rangle^{-3} \in (\mathcal{L}_{\frac{d}{2},\infty})_0, \tag{4.28}$$

for all $k = 1, \ldots, d-1$, and $j = k+1, \ldots, d$.

Fix $k = 1, \ldots, d-1$, and $j = k+1, \ldots, d$ and let $f \in C^\infty_{\mathrm{com}}(\mathbb{R}^d)$ satisfying either $f\partial_k\phi \neq 0$ or $f\partial_j\phi \neq 0$ on $\mathrm{supp}(f)$. By Proposition 2.56 (*ii*) (with $p = 1$, $\delta = d$), we have that

$$\langle\nabla\rangle^{-d} M_{f^2} \in \mathcal{L}_{1,\infty}. \tag{4.29}$$

For brevity, define the operator $T_{j,k}$ on the domain $W_2^d(\mathbb{R}^d)$ by

$$T_{j,k} := \langle\nabla\rangle^{d-1}(\partial_k M_{f^2\partial_j\phi} - \partial_j M_{f^2\partial_k\phi}).$$

If $d > 2$, then Proposition 2.56 (with $p = \frac{d}{d-2}$) implies that

$$\langle\nabla\rangle^{2-d} M_{f^2} \in \mathcal{L}_{\frac{d}{d-2},\infty}.$$

Therefore,

$$T_{j,k} \in \begin{cases} \mathcal{L}_{\frac{d}{d-2},\infty}\big(L_2(\mathbb{R}^d)\big), & \text{if } d > 2 \\ \mathcal{B}\big(L_2(\mathbb{R}^d)\big), & \text{if } d = 2 \end{cases}.$$

By the Hölder inequality for weak Schatten classes (see (2.23) above), the latter inclusion together with the assumption (4.28) implies that

$$\Phi_{j,k}T_{j,k} \in (\mathcal{L}_{1,\infty})_0, \quad \text{for all } d \geq 2,$$

and therefore that the Dixmier trace

$$\mathrm{Tr}_\omega(\Phi_{j,k}T_{j,k}) = 0, \tag{4.30}$$

for any extended limit ω on $\ell_\infty(\mathbb{N})$. However, we claim that $\mathrm{Tr}_\omega(\Phi_{j,k}T_{j,k})$ is not necessarily zero.

By the definitions of $\Phi_{j,k}$ and $T_{j,k}$ we have

$$\begin{aligned} &\mathrm{Tr}_\omega(\Phi_{j,k}T_{j,k}) \\ &\quad = \mathrm{Tr}_\omega\left(M_{\partial_j\phi}\partial_k^2\langle\nabla\rangle^{-d-2}M_{f^2\partial_j\phi}\right) - \mathrm{Tr}_\omega\left(M_{\partial_j\phi}\partial_k\partial_j\langle\nabla\rangle^{-d-2}M_{f^2\partial_k\phi}\right) \\ &\qquad - \mathrm{Tr}_\omega\left(M_{\partial_k\phi}\partial_k^2\langle\nabla\rangle^{-d-2}M_{f^2\partial_j\phi}\right) + \mathrm{Tr}_\omega\left(M_{\partial_k\phi}\partial_j^2\langle\nabla\rangle^{-d-2}M_{f^2\partial_k\phi}\right). \end{aligned} \tag{4.31}$$

Consider the first term on the right-hand side of the above. Since $\langle\nabla\rangle^{-d}M_{f^2}$ and $M_{f^2}\langle\nabla\rangle^{-d}$ both belong to $\mathcal{L}_{1,\infty}$ by Proposition 2.56, the cyclicity of the trace Tr_ω (see Proposition 2.25 above) gives the identity

$$\mathrm{Tr}_\omega\left(M_{\partial_j\phi}\partial_k^2\langle\nabla\rangle^{-d-2}M_{f^2\partial_j\phi}\right) = \mathrm{Tr}_\omega\left(M_{(f\partial_j\phi)^2}\partial_k^2\langle\nabla\rangle^{-d-2}\right). \tag{4.32}$$

Using the fact that

$$(-\Delta)\langle\nabla\rangle^{-d-2} = (-\Delta)(1-\Delta)^{-\frac{d+2}{2}} = (1-\Delta)^{-\frac{d}{2}} - (1-\Delta)^{-\frac{d+2}{2}} = \langle\nabla\rangle^{-d} - \langle\nabla\rangle^{-d-2},$$

we have

$$\mathrm{Tr}_\omega\left(M_{(f\partial_j\phi)^2}\partial_k^2\langle\nabla\rangle^{-d-2}\right) = \mathrm{Tr}_\omega\left(M_{(f\partial_j\phi)^2}\frac{\partial_k^2}{(-\Delta)}\langle\nabla\rangle^{-d}\right) - \tau\Big(M_{(f\partial_j\phi)^2}\frac{\partial_k^2}{(-\Delta)}\langle\nabla\rangle^{-d-2}\Big).$$

Note that, by Proposition 4.3 (*ii*) (with $\lambda = 0$, $p = 1$ and $\alpha = d+2$), we have that $M_f\langle\nabla\rangle^{-d-2} \in \mathcal{L}_1$. Hence, $M_{(f\partial_j\phi)^2}\frac{\partial_k^2}{(-\Delta)}\langle\nabla\rangle^{-d-2}$ is also trace-class, so the singular trace Tr_ω vanishes on this operator, and

$$\mathrm{Tr}_\omega\left(M_{(f\partial_j\phi)^2}\partial_k^2\langle\nabla\rangle^{-d-2}\right) = \mathrm{Tr}_\omega\left(M_{(f\partial_j\phi)^2}\frac{\partial_k^2}{(-\Delta)}\langle\nabla\rangle^{-d}\right). \tag{4.33}$$

Hence, by Lemma 3.15, we infer that $\Phi_{j,k}T_{j,k}$ is Dixmier measurable, and that

$$\mathrm{Tr}_\omega(\Phi_{j,k}T_{j,k}) = C_d\Big(\int_{\mathbb{R}^d}(f\partial_j\phi)^2(\mathbf{t})\,\mathrm{d}\mathbf{t} + \int_{\mathbb{R}^d}(f\partial_k\phi)^2(\mathbf{t})\,\mathrm{d}\mathbf{t}\Big),$$

where $C_d > 0$.

However, the choice of f guarantees that either $\int_{\mathbb{R}^d}(f\partial_j\phi)^2(\mathbf{t})\,\mathrm{d}\mathbf{t}$ or $\int_{\mathbb{R}^d}(f\partial_k\phi)^2(\mathbf{t})\,\mathrm{d}\mathbf{t}$ is nonzero (or they are both nonzero, but have the same sign). Therefore, we see that

$$\mathrm{Tr}_\omega(\Phi_{j,k}T_{j,k}) \neq 0,$$

which contradicts the equality (4.30) obtained above. Thus, we conclude that the operator $\mathrm{g}(\mathcal{D}+\mathbb{I}\otimes M_\phi)-\mathrm{g}(\mathcal{D})$ must not belong to $(\mathcal{L}_{\frac{d}{2},\infty})_0$.

(ii). Suppose $\mathbf{A}\neq 0$. Again arguing by contradiction, we assume to the contrary that $\mathrm{g}(\mathcal{D}+V)-\mathrm{g}(\mathcal{D})\in(\mathcal{L}_{d,\infty})_0$. By Proposition 4.15, this would imply that

$$\sum_{j=1}^{d}\gamma_j\otimes\Psi_j\in(\mathcal{L}_{d,\infty})_0.$$

Hence, by Lemma 2.12 (i), we must have that

$$\Psi_j=\sum_{k\neq j}(M_{a_k}\partial_j\partial_k-M_{a_j}\partial_k^2)\langle\nabla\rangle^{-3}\in(\mathcal{L}_{d,\infty})_0,$$

for all $j=1,\dots,d$.

Since $\mathbf{A}\neq 0$, it follows that there exists some $j=1,\dots,d$ such that $a_j\neq 0$; in the following, we fix such j. Additionally, let $f\in C^\infty_{\mathrm{com}}(\mathbb{R}^d)$ such that $fa_j\neq 0$ on $\mathrm{supp}(f)$, and define the bounded operator

$$S_j:=\langle\nabla\rangle^{1-d}M_{f^2a_j}$$

on $L_2(\mathbb{R}^d)$. Arguing in an analogous manner to the proof of (i) above, one can show that $\Psi_jS_j\in(\mathcal{L}_{1,\infty})_0$, and therefore,

$$\mathrm{Tr}_\omega(\Psi_jS_j)=0,$$

for any extended limit ω on $\ell_\infty(\mathbb{N})$.

On the other hand, continuing to argue similarly to the proof of (i) above, we have that

$$\begin{aligned}\mathrm{Tr}_\omega(\Psi_jS_j)&=\sum_{k\neq j}\mathrm{Tr}_\omega\left(M_{f^2a_ka_j}\partial_k\partial_j\langle\nabla\rangle^{-d-2}\right)-\sum_{k\neq j}\mathrm{Tr}_\omega\left(M_{(fa_j)^2}\partial_k^2\langle\nabla\rangle^{-d-2}\right)\\&=\sum_{k\neq j}\mathrm{Tr}_\omega\left(M_{f^2a_ka_j}\partial_k\partial_j(-\Delta)^{-1}\langle\nabla\rangle^{-d}\right)-\sum_{k\neq j}\mathrm{Tr}_\omega\left(M_{(fa_j)^2}\partial_k^2(-\Delta)^{-1}\langle\nabla\rangle^{-d}\right)\end{aligned}$$

Hence, Lemma 3.15 implies that Ψ_jS_j is Dixmier measurable, and that

$$\mathrm{Tr}_\omega(\Psi_jS_j)=-(d-1)C_d\int_{\mathbb{R}^d}(fa_j)^2(\mathbf{t})\,\mathrm{d}\mathbf{t},$$

where $C_d>0$. However, the choice of f guarantees that $\int_{\mathbb{R}^d}(fa_j)^2(\mathbf{t})\,\mathrm{d}\mathbf{t}>0$, and therefore that $\mathrm{Tr}_\omega(\Psi_jS_j)\neq 0$, which is a contradiction. □

4.2 Lipschitz-type estimates for Schwartz antiderivatives of the Dirac operator

In this section, we prove the main result of this chapter, Theorem 4.21 below. We begin with some auxiliary lemmas.

Lemma 4.18. *If $\phi, a_1, \ldots, a_d \in (W^3_{\frac{d}{2}} \cap W^3_\infty)(\mathbb{R}^d)$, then*

$$\mathrm{g}^2(\mathcal{D}+V) - \mathrm{g}^2(\mathcal{D}) \in \mathcal{L}_{\frac{d}{2}}.$$

Proof. First, observe that $\mathrm{g}^2(t) = t^2\langle t\rangle^{-2} = 1 - \langle t\rangle^{-2}$, for all $t \in \mathbb{R}$, so appealing to the second resolvent identity yields the equation

$$\begin{aligned}\mathrm{g}^2(\mathcal{D}+V) - \mathrm{g}^2(\mathcal{D}) &= \langle\mathcal{D}\rangle^{-2} - \langle\mathcal{D}+V\rangle^{-2} = \langle\mathcal{D}\rangle^{-2}\big((\mathcal{D}+V)^2 - \mathcal{D}^2\big)\langle\mathcal{D}+V\rangle^{-2}\\ &= \langle\mathcal{D}\rangle^{-2}(\mathcal{D}V + V\mathcal{D} + V^2)\langle\mathcal{D}\rangle^{-2}\cdot\langle\mathcal{D}\rangle^{2}\langle\mathcal{D}+V\rangle^{-2}.\end{aligned}$$

Since V is bounded, we have by [19, Appendix B-Lemma 6] that $\langle\mathcal{D}\rangle^2\langle\mathcal{D}+V\rangle^{-2}$ is a bounded operator on $L_2(\mathbb{R}^d)^{N_d}$, and therefore it suffices to show that the operators

$$\langle\mathcal{D}\rangle^{-2}\mathcal{D}V\langle\mathcal{D}\rangle^{-2}, \quad \langle\mathcal{D}\rangle^{-2}V\mathcal{D}\langle\mathcal{D}\rangle^{-2}, \quad \langle\mathcal{D}\rangle^{-2}V^2\langle\mathcal{D}\rangle^{-2}$$

are in $\mathcal{L}_{\frac{d}{2}}$. We show this only for the first operator, since the others can be treated similarly.

By Theorem 2.20 above, we have

$$\big\|\langle\mathcal{D}\rangle^{-1}V\langle\mathcal{D}\rangle^{-2}\big\|_{\frac{d}{2}} \le \big\|V\langle\mathcal{D}\rangle^{-3}\big\|_{\frac{d}{2}}.$$

Furthermore, since

$$V = \mathbb{I}\otimes M_\phi - \sum_{j=1}^d \gamma_j \otimes M_{a_j},$$

we have by Proposition 4.3 (with $\lambda = 0$, $p = \frac{d}{2}$, $\alpha = 3$) that

$$\begin{aligned}\big\|V\langle\mathcal{D}\rangle^{-3}\big\|_{\frac{d}{2}} &\le \begin{cases}\mathrm{const}\cdot\Big(\|\phi\|_{\frac{d}{2}} + \sum_{j=1}^d \|a_j\|_{\frac{d}{2}}\Big), & \text{if } d \ge 4,\\ \mathrm{const}\cdot\Big(\|\phi\|_{W^3_{\frac{3}{2}}} + \sum_{j=1}^d \|a_j\|_{W^3_{\frac{3}{2}}}\Big), & \text{if } d = 3,\\ \mathrm{const}\cdot\Big(\|\phi\|_{W^2_1} + \sum_{j=1}^d \|a_j\|_{W^2_1}\Big), & \text{if } d = 2,\end{cases}\\ &< \infty,\end{aligned}$$

which concludes the proof. □

Lemma 4.19. *Suppose $\phi, a_1, \ldots, a_d \in (W^3_{\frac{d}{2}} \cap W^3_\infty)(\mathbb{R}^d)$. If $f_0 \in C^2_{\mathrm{b}}(\mathbb{R})$ is an even function, then*

$$f_0(\mathcal{D}+V) - f_0(\mathcal{D}) \in \mathcal{L}_{\frac{d}{2}}.$$

Proof. Since g^2 is an even function, and since $\mathrm{g}^2 : [0,\infty) \to [0,1)$ is injective, we may write $f_0 = h \circ \mathrm{g}^2$, where $h := f_0 \circ \mathrm{g}^{-2} : [0,1) \to \mathbb{R}$ is also a C^2-function. Hence, by Theorem

2.66 above, we have

$$\begin{aligned} f_0(\mathcal{D}+V) - f_0(\mathcal{D}) &= h\big(\mathrm{g}^2(\mathcal{D}+V)\big) - h\big(\mathrm{g}^2(\mathcal{D})\big) \\ &= \mathcal{J}_{h^{[1]}}^{\mathrm{g}^2(\mathcal{D}+V),\mathrm{g}^2(\mathcal{D})}\big(\mathrm{g}^2(\mathcal{D}+V) - \mathrm{g}^2(\mathcal{D})\big) \in \mathcal{L}_{\frac{d}{2}}, \end{aligned}$$

since $\mathrm{g}^2(\mathcal{D}+V) - \mathrm{g}^2(\mathcal{D}) \in \mathcal{L}_{\frac{d}{2}}$ by Lemma 4.18. □

Lemma 4.20. *Suppose $\phi \in (W^5_{\frac{d}{2}} \cap W^5_\infty)(\mathbb{R}^d)$ and $\mathbf{A} \in (W^2_{\frac{d}{2}} \cap W^2_\infty)(\mathbb{R}^d)^d$.*

(*i*) *If $\mathbf{A} = 0$, then $\big(\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})\big)\langle\mathcal{D}\rangle^{-2} \in \mathcal{L}_{\frac{d}{2}}$.*

(*ii*) *If $\mathbf{A} \neq 0$, then $\big(\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})\big)\langle\mathcal{D}\rangle^{-2} \in \mathcal{L}_d$.*

Proof. (*i*). Suppose $\mathbf{A} = 0$. By Proposition 4.11, it suffices to show that

$$\Phi_{j,k}\langle\nabla\rangle^{-2} = (M_{\partial_j\phi}\partial_k - M_{\partial_k\phi}\partial_j)\langle\nabla\rangle^{-5} \in \mathcal{L}_{\frac{d}{2}}, \quad \text{for all } j > k.$$

Hence, it suffices to show that $M_{\partial_j\phi}\langle\nabla\rangle^{-4} \in \mathcal{L}_{\frac{d}{2}}$, for all $j = 1, \ldots, d$.

Suppose $d \geq 4$. Since $\partial_j\phi \in L_{\frac{d}{2}}(\mathbb{R}^d)$ by assumption, Proposition 4.3 (*i*) (with $\lambda = 0$, $p = \frac{d}{2}$, $\alpha = 4$) implies that $M_{\partial_j\phi}\langle\nabla\rangle^{-4} \in \mathcal{L}_{\frac{d}{2}}$.

Next, suppose $d = 2, 3$. Since $\partial_j\phi \in W^d_{\frac{d}{2}}(\mathbb{R}^d)$ by assumption, Proposition 4.3 (*ii*) (with $\lambda = 0$, $p = \frac{d}{2}$, $\alpha = 4$) implies that $M_{\partial_j\phi}\langle\nabla\rangle^{-4} \in \mathcal{L}_{\frac{d}{2}}$, as required.

(*ii*). Suppose $\mathbf{A} \neq 0$. By Proposition 4.15 and similar reasoning to the proof of part (*i*), it suffices to show that $M_{a_j}\langle\nabla\rangle^{-3} \in \mathcal{L}_d$, for all $j = 1, \ldots, d$. However, this follows immediately from Proposition 4.3 (*i*) (with $\lambda = 0$, $p = d$, $\alpha = 3$). □

Now, in the following, let f be a real-valued function on $\mathbb{R}$ such that $f' \in \mathcal{S}(\mathbb{R})$. For brevity, we denote the limits of f at infinity by

$$f(+\infty) := \lim_{t\to\infty} f(t), \qquad f(-\infty) := \lim_{t\to-\infty} f(t),$$

and assume that $f(+\infty) \neq f(-\infty)$. Moreover, we define the functions $f_0, f_1, f_{0,\mathrm{m}}, f_{1,\mathrm{m}}$ on $\mathbb{R}$ by

$$f_0(t) := \frac{f(t) + f(-t)}{2}, \qquad f_1(t) := \frac{f(t) - f(-t)}{2},$$

$$f_{0,\mathrm{m}}(t) := f_0(t) - f_0(+\infty), \qquad f_{1,\mathrm{m}}(t) := \begin{cases} \dfrac{f_1(t)}{\mathrm{g}(t) f_1(+\infty)} - 1, & \text{if } t \neq 0, \\ -1, & \text{if } t = 0. \end{cases}$$

One can check that $f_{0,\mathrm{m}}, f_{1,\mathrm{m}} \in \mathcal{S}(\mathbb{R})$. By construction,

$$\begin{aligned} f(t) = f_0(t) + f_1(t) &= f_0(+\infty) + \big(f_0(t) - f_0(+\infty)\big) + \mathrm{g}(t)\Big(\frac{f_1(t)}{\mathrm{g}(t) f_1(+\infty)}\Big) f_1(+\infty) \\ &= f_0(+\infty) + f_{0,\mathrm{m}}(t) + \mathrm{g}(t)\big(1 + f_{1,\mathrm{m}}(t)\big) f_1(+\infty), \quad t \in \mathbb{R} \setminus \{0\}. \end{aligned} \tag{4.34}$$

Theorem 4.21. *Suppose* $\phi \in (W^5_{\frac{d}{2}} \cap W^5_\infty)(\mathbb{R}^d)$ *and* $\mathbf{A} \in (W^2_{\frac{d}{2}} \cap W^2_\infty)(\mathbb{R}^d)^d$. *Suppose* $f : \mathbb{R} \to \mathbb{R}$ *is a function such that* $f' \in \mathcal{S}(\mathbb{R})$ *and* $f(-\infty) \neq f(+\infty)$.

(*i*) *If* $\mathbf{A} = 0$ *and* $\phi \neq 0$, *then* $f(\mathcal{D}+V) - f(\mathcal{D}) \in \mathcal{L}_{\frac{d}{2},\infty} \setminus (\mathcal{L}_{\frac{d}{2},\infty})_0$.

(*ii*) *If* $\mathbf{A} \neq 0$, *then* $f(\mathcal{D}+V) - f(\mathcal{D}) \in \mathcal{L}_{d,\infty} \setminus (\mathcal{L}_{d,\infty})_0$.

Proof. Since $f_{0,\mathrm{m}} \in C^2_{\mathrm{b}}(\mathbb{R})$ is even, Lemma 4.19 implies that

$$f_{0,\mathrm{m}}(\mathcal{D}+V) - f_{0,\mathrm{m}}(\mathcal{D}) \in \mathcal{L}_{\frac{d}{2}}.$$

Furthermore,

$$\begin{aligned}&\mathrm{g}(\mathcal{D}+V)\big(1+f_{1,\mathrm{m}}(\mathcal{D}+V)\big) - \mathrm{g}(\mathcal{D})\big(1+f_{1,\mathrm{m}}(\mathcal{D})\big)\\ &\qquad = \mathrm{g}(\mathcal{D}+V)\big(f_{1,\mathrm{m}}(\mathcal{D}+V) - f_{1,\mathrm{m}}(\mathcal{D})\big) + \big(\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})\big)\big(1+f_{1,\mathrm{m}}(\mathcal{D})\big),\end{aligned}$$

and, since $f_{1,\mathrm{m}} \in C^2_{\mathrm{b}}(\mathbb{R})$ and is even, again using Lemma 4.19, we have that

$$\mathrm{g}(\mathcal{D}+V)\big(f_{1,\mathrm{m}}(\mathcal{D}+V) - f_{1,\mathrm{m}}(\mathcal{D})\big) \in \mathcal{L}_{\frac{d}{2}}.$$

Hence,

$$f(\mathcal{D}+V) - f(\mathcal{D}) \overset{(4.34)}{\in} f_1(+\infty)\big(\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})\big)\big(1+f_{1,\mathrm{m}}(\mathcal{D})\big) + \mathcal{L}_{\frac{d}{2}}.$$

Additionally, observe that the function given by $\theta_f(t) := f_{1,\mathrm{m}}(t)\langle t\rangle^2$, for $t \in \mathbb{R}$, is bounded. Hence, by Lemma 4.20, we observe that

$$\big(\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})\big)f_{1,\mathrm{m}}(\mathcal{D}) = \big(\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D})\big)\langle\mathcal{D}\rangle^{-2}\theta_f(\mathcal{D}) \in \begin{cases}\mathcal{L}_{\frac{d}{2}}, & \text{if } \mathbf{A} = 0,\\ \mathcal{L}_d, & \text{if } \mathbf{A} \neq 0,\end{cases}$$

and thus,

$$f(\mathcal{D}+V) - f(\mathcal{D}) \in \begin{cases}\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) + \mathcal{L}_{\frac{d}{2}}, & \text{if } \mathbf{A} = 0 \text{ and } \phi \neq 0,\\ \mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) + \mathcal{L}_d, & \text{if } \mathbf{A} \neq 0.\end{cases}$$

Finally, by Theorems 4.16 and 4.17, we have that

$$\mathrm{g}(\mathcal{D}+V) - \mathrm{g}(\mathcal{D}) \in \begin{cases}\mathcal{L}_{\frac{d}{2},\infty} \setminus (\mathcal{L}_{\frac{d}{2},\infty})_0, & \text{if } \mathbf{A} = 0 \text{ and } \phi \neq 0,\\ \mathcal{L}_{d,\infty} \setminus (\mathcal{L}_{d,\infty})_0, & \text{if } \mathbf{A} \neq 0,\end{cases}$$

so

$$f(\mathcal{D}+V) - f(\mathcal{D}) \in \begin{cases}\mathcal{L}_{\frac{d}{2},\infty} \setminus (\mathcal{L}_{\frac{d}{2},\infty})_0, & \text{if } \mathbf{A} = 0 \text{ and } \phi \neq 0,\\ \mathcal{L}_{d,\infty} \setminus (\mathcal{L}_{d,\infty})_0, & \text{if } \mathbf{A} \neq 0.\end{cases}$$

□

Appendix A

Miscellaneous integrals and estimates

A.1 Asymptotics of the Sobolev norm of g_p

In this appendix, we calculate the behaviour of the Sobolev norm $\|g_p\|_{W_2^n}$ as $p \downarrow 1$, for $n \in \mathbb{N}$, where g_p is the Schwartz function on $\mathbb{R}$ defined in Section 3.1 above by the expression

$$g_p(t) \coloneqq \begin{cases} \frac{1}{2}\Big(1 - \coth\Big(\frac{t}{2}\Big)\tanh\Big(\frac{(p-1)t}{2}\Big)\Big), & \text{if } t \neq 0, \\ 1 - \frac{p}{2}, & \text{if } t = 0. \end{cases}$$

Let $n \in \mathbb{N}$ and $p \geq 1$. In the following, for $-\infty \leq a < b \leq \infty$, we recall that the Sobolev space of p-integrable functions on the interval (a, b) is defined by

$$W_p^n(a,b) \coloneqq \Big\{ f \in L_p(a,b) \ : \ f^{(j)} \in L_p(a,b), \text{ for all } j = 1, \dots, n \Big\},$$

where $f^{(j)} \coloneqq \dfrac{\mathrm{d}^j f}{\mathrm{d}x^j}$ is interpreted as a weak derivative, with corresponding norm given by

$$\|f\|_{W_p^n(a,b)} \coloneqq \sum_{j=0}^{n} \|f^{(j)}\|_{L_p(a,b)}, \quad f \in W_p^n(a,b).$$

Lemma A.1. *For $n \in \mathbb{N}$, we have*

$$\|g_p\|_{W_\infty^n(0,1)} = \mathcal{O}(1), \quad p \downarrow 1.$$

Proof. For $u > 0$, let δ_u be the dilation operator on $C^\infty(0,\infty)$ defined by

$$(\delta_u f)(t) \coloneqq f(ut), \qquad \text{for } f \in C^\infty(0,\infty),\ t > 0.$$

For $p > 1$, we write

$$g_p = h \cdot \big(f - (p-1)(\delta_{p-1} f)\big),$$

where
$$h(t)=\frac{t}{2}\coth\Big(\frac{t}{2}\Big),\quad f(t)=\frac{1}{t}\tanh\Big(\frac{t}{2}\Big),\quad t\in\mathbb{R}.$$
By the Leibniz rule, we have
$$\begin{aligned}\|g_p\|_{W^n_\infty(0,1)}&\le\Big\|h\cdot\big(f-(p-1)(\delta_{p-1}f)\big)\Big\|_{W^n_\infty(0,1)}\\&\le\|h\|_{W^n_\infty(0,1)}\big\|f-(p-1)(\delta_{p-1}f)\big\|_{W^n_\infty(0,1)}.\end{aligned}$$
For $0\le k\le n$, we have
$$\big(f-(p-1)(\delta_{p-1}f)\big)^{(k)}=f^{(k)}-(p-1)^{k+1}\delta_{p-1}(f^{(k)}).$$
Hence,
$$\Big\|\big(f-(p-1)(\delta_{p-1}f)\big)^{(k)}\Big\|_\infty\le\big(1+(p-1)^{k+1}\big)\|f^{(k)}\|_\infty.$$ □

Lemma A.2. *For $n\in\mathbb{N}$, we have*
$$\|g_p\|_{W^n_2(1,\infty)}=\mathcal{O}\big((p-1)^{-\frac12}\big),\quad p\downarrow 1.$$

Proof. Let $(\delta_u f)(t)=f(ut)$. We write
$$g_p=h\cdot(f-\delta_{p-1}f),$$
where
$$h(t)=\frac{1}{2}\coth\Big(\frac{t}{2}\Big),\quad f(t)=\tanh\Big(\frac{t}{2}\Big),\quad t\in\mathbb{R}.$$
By Leibniz rule, we have
$$\|g_p\|_{W^n_2(1,\infty)}\le\|h\|_{W^n_\infty(1,\infty)}\|f-\delta_{p-1}f\|_{W^n_2(1,\infty)}.$$

For $0\le k\le n$, we have
$$(f-\delta_{p-1}f)^{(k)}=f^{(k)}-(p-1)^k\delta_{p-1}(f^{(k)}).$$

Hence,
$$\begin{aligned}\big\|(f-\delta_{p-1}f)^{(k)}\big\|_{L_2(1,\infty)}&\le\|f^{(k)}\|_{L_2(1,\infty)}+(p-1)^k\big\|\delta_{p-1}(f^{(k)})\big\|_{L_2(1,\infty)}\\&\le\big(1+(p-1)^{k-\frac12}\big)\cdot\|f^{(k)}\|_{L_2(0,\infty)}.\end{aligned}$$ □

Lemma A.3. *For g_p defined as above, $\|g_p\|_{W^n_2}=\mathcal{O}\big((p-1)^{-\frac12}\big)$ as $p\downarrow 1$.*

Proof. Since g_p is even, we have
$$\|g_p\|_{W^n_2}\le 2\big(\|g_p\|_{W^n_2(0,1)}+\|g_p\|_{W^n_2(1,\infty)}\big)\le 2\big(\|g_p\|_{W^n_\infty(0,1)}+\|g_p\|_{W^n_2(1,\infty)}\big).$$

The assertion follows from the preceding lemmas. □

A.2 Calculation of Bochner integrals

Observe that, when $\alpha > -1$, $\beta > \alpha + 1$, and A is a positive operator, we have

$$\int_0^\infty \lambda^\alpha (1+\lambda+A)^{-\beta} \,\mathrm{d}\lambda = \mathrm{B}(\alpha+1; \beta-\alpha-1)(1+A)^{\alpha-\beta+1}, \tag{A.1}$$

where $\mathrm{B}(\cdot\,;\cdot)$ denotes the Beta function [1, 6.2.1].

Proof of Lemma 4.6. Appealing to the definition of $\mathcal{R}_{0,\lambda}$ (see (4.1)), and since

$$\frac{1}{\big(t+i(1+\lambda)^{\frac{1}{2}}\big)^3} = \frac{t^3 - 3t(1+\lambda)}{(1+\lambda+t^2)^3} + i\frac{(1+\lambda)^{\frac{3}{2}} - 3t^2(1+\lambda)^{\frac{1}{2}}}{(1+\lambda+t^2)^3}, \quad \text{for all } t \in \mathbb{R},$$

we obtain the expression

$$\mathfrak{Re}(\mathcal{R}_{0,\lambda}^3) = \big(\mathcal{D}^3 - 3\mathcal{D}(1+\lambda)\big)(1+\lambda+\mathcal{D}^2)^{-3}.$$

Hence, by (A.1), we obtain the identity

$$\begin{aligned}
&\Big(\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\,\mathfrak{Re}(\mathcal{R}_{0,\lambda}^3)\Big) \\
&\qquad = (\mathcal{D}^3 - 3\mathcal{D})\int_0^\infty \lambda^{-\frac{1}{2}}(1+\lambda+\mathcal{D}^2)^{-3}\,\mathrm{d}\lambda - 3\mathcal{D}\int_0^\infty \lambda^{\frac{1}{2}}(1+\lambda+\mathcal{D}^2)^{-3}\,\mathrm{d}\lambda \\
&\qquad \overset{\text{(A.1)}}{=} \frac{3\pi}{8}(\mathcal{D}^3 - 3\mathcal{D})(1+\mathcal{D}^2)^{-\frac{5}{2}} - \frac{3\pi}{8}\mathcal{D}(1+\mathcal{D}^2)^{-\frac{3}{2}} = -\frac{3\pi}{2}\mathcal{D}(1+\mathcal{D}^2)^{-\frac{5}{2}}.
\end{aligned}$$

□

Proof of Lemma 4.9. By calculating the real and imaginary parts of the complex numbers $\big(t+i(1+\lambda)^{\frac{1}{2}}\big)^{-1}$, $\big(t+i(1+\lambda)^{\frac{1}{2}}\big)^{-2}$, $t \in \mathbb{R}$, we acquire the expressions

$$\begin{aligned}
\mathcal{R}_{0,\lambda} &= \big(\mathcal{D} - i(1+\lambda)^{\frac{1}{2}}\big)(1+\lambda+\mathcal{D}^2)^{-1}, \\
\mathcal{R}_{0,\lambda}^2 &= \big(\mathcal{D}^2 - 2i(1+\lambda)^{\frac{1}{2}}\mathcal{D} - (1+\lambda)\big)(1+\lambda+\mathcal{D}^2)^{-2}.
\end{aligned} \tag{A.2}$$

(i) Fixing $k \in \{1,\dots,d\}$, by expanding and cancelling similar terms, we get

$$\begin{aligned}
&\mathcal{R}_{0,\lambda}(\gamma_k\otimes 1)\mathcal{R}_{0,\lambda}^2 + \mathcal{R}_{0,\lambda}^*(\gamma_k\otimes 1)(\mathcal{R}_{0,\lambda}^*)^2 \\
&\overset{\text{(A.2)}}{=} \big(\mathcal{D} - i(1+\lambda)^{\frac{1}{2}}\big)(1+\lambda+\mathcal{D}^2)^{-1}(\gamma_k\otimes 1)\big(\mathcal{D}^2 - 2i(1+\lambda)^{\frac{1}{2}}\mathcal{D} - (1+\lambda)\big)(1+\lambda+\mathcal{D}^2)^{-2} \\
&\quad + \big(\mathcal{D} + i(1+\lambda)^{\frac{1}{2}}\big)(1+\lambda+\mathcal{D}^2)^{-1}(\gamma_k\otimes 1)\big(\mathcal{D}^2 + 2i(1+\lambda)^{\frac{1}{2}}\mathcal{D} - (1+\lambda)\big)(1+\lambda+\mathcal{D}^2)^{-2} \\
&= 2\mathcal{D}(1+\lambda+\mathcal{D}^2)^{-1}(\gamma_k\otimes 1)\big(\mathcal{D}^2 - (1+\lambda)\big)(1+\lambda+\mathcal{D}^2)^{-2} \\
&\qquad - 4(1+\lambda)(1+\lambda+\mathcal{D}^2)^{-1}(\gamma_k\otimes 1)\mathcal{D}(1+\lambda+\mathcal{D}^2)^{-2} \\
&= 2\big(\mathcal{D}(\gamma_k\otimes 1)(\mathcal{D}^2-1) - \mathcal{D}(\gamma_k\otimes 1)\lambda - 2(\gamma_k\otimes 1)\mathcal{D}(1+\lambda)\big)(1+\lambda+\mathcal{D}^2)^{-3},
\end{aligned}$$

where in the last line we used the fact that $\mathcal{D}^2$ commutes with $\gamma_k\otimes 1$. Hence, for each

$k \in \{1, \dots, d\}$, by (A.1), we get that

$$\begin{aligned}
&\frac{1}{2}\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\big(\mathcal{R}_{0,\lambda}(\gamma_k\otimes 1)\mathcal{R}_{0,\lambda}^2 + \mathcal{R}_{0,\lambda}^*(\gamma_k\otimes 1)(\mathcal{R}_{0,\lambda}^*)^2\big)\\
&\quad = \big((1+\mathcal{D}^2)-2\big)\Big(\int_0^\infty \lambda^{-\frac{1}{2}}(1+\lambda+\mathcal{D}^2)^{-3}\,\mathrm{d}\lambda\Big)\mathcal{D}(\gamma_k\otimes 1)\\
&\qquad - \Big(\int_0^\infty \lambda^{\frac{1}{2}}(1+\lambda+\mathcal{D}^2)^{-3}\,\mathrm{d}\lambda\Big)\mathcal{D}(\gamma_k\otimes 1)\\
&\qquad - 2(\gamma_k\otimes 1)\mathcal{D}\Big(\int_0^\infty (\lambda^{-\frac{1}{2}}+\lambda^{\frac{1}{2}})(1+\lambda+\mathcal{D}^2)^{-3}\,\mathrm{d}\lambda\Big)\\
&\quad \overset{(A.1)}{=} \frac{3\pi}{8}\big((1+\mathcal{D}^2)-2\big)(1+\mathcal{D}^2)^{-\frac{5}{2}}\mathcal{D}(\gamma_k\otimes 1) - \frac{\pi}{8}(1+\mathcal{D}^2)^{-\frac{3}{2}}\mathcal{D}(\gamma_k\otimes 1)\\
&\qquad - \frac{3\pi}{4}(\gamma_k\otimes 1)\mathcal{D}(1+\mathcal{D}^2)^{-\frac{5}{2}} - \frac{\pi}{4}(\gamma_k\otimes 1)\mathcal{D}(1+\mathcal{D}^2)^{-\frac{3}{2}}\\
&\quad = \frac{\pi}{4}\big(\mathcal{D}(\gamma_k\otimes 1)-(\gamma_k\otimes 1)\mathcal{D}\big)(1+\mathcal{D}^2)^{-\frac{3}{2}} - \frac{3\pi}{4}\big(\mathcal{D}(\gamma_k\otimes 1)+(\gamma_k\otimes 1)\mathcal{D}\big)(1+\mathcal{D}^2)^{-\frac{5}{2}}.
\end{aligned}$$

(ii). Note that, by (A.2), we obtain

$$\begin{aligned}
\frac{1}{2}\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\,\mathfrak{Re}(\mathcal{R}_{0,\lambda}^2) &= \int_0^\infty \lambda^{-\frac{1}{2}}\big(\mathcal{D}^2-(1+\lambda)\big)(1+\lambda+\mathcal{D}^2)^{-2}\,\mathrm{d}\lambda\\
&= (\mathcal{D}^2-1)\int_0^\infty \lambda^{-\frac{1}{2}}(1+\lambda+\mathcal{D}^2)^{-2}\,\mathrm{d}\lambda - \int_0^\infty \lambda^{\frac{1}{2}}(1+\lambda+\mathcal{D}^2)^{-2}\,\mathrm{d}\lambda\\
&\overset{(A.1)}{=} \frac{\pi}{2}(\mathcal{D}^2-1)(1+\mathcal{D}^2)^{-\frac{3}{2}} - \frac{\pi}{2}(1+\mathcal{D}^2)^{-\frac{1}{2}} = -\pi(1+\mathcal{D}^2)^{-\frac{3}{2}}.
\end{aligned}$$
□

Proof of Lemma 4.14. Using (A.2), and by expanding and cancelling similar terms, we obtain

$$\begin{aligned}
&\mathfrak{Re}\,\big(\mathcal{R}_{0,\lambda}(\gamma_j\otimes 1)\mathcal{R}_{0,\lambda}\big)\\
&\quad = \frac{1}{2}\big(\mathcal{D}-i(1+\lambda)^{\frac{1}{2}}\big)(1+\lambda+\mathcal{D}^2)^{-1}(\gamma_j\otimes 1)\big(\mathcal{D}-i(1+\lambda)^{\frac{1}{2}}\big)(1+\lambda+\mathcal{D}^2)^{-1}\\
&\qquad + \frac{1}{2}\big(\mathcal{D}+i(1+\lambda)^{\frac{1}{2}}\big)(1+\lambda+\mathcal{D}^2)^{-1}(\gamma_j\otimes 1)\big(\mathcal{D}+i(1+\lambda)^{\frac{1}{2}}\big)(1+\lambda+\mathcal{D}^2)^{-1}\\
&\quad = \big(\mathcal{D}(\gamma_j\otimes 1)\mathcal{D}-(1+\lambda)\big)(1+\lambda+\mathcal{D}^2)^{-2}\\
&\quad \overset{(4.23)}{=} -\big((\gamma_j\otimes 1)\mathcal{D}_j\mathcal{D}+(1+\lambda)\big)(1+\lambda+\mathcal{D}^2)^{-2}.
\end{aligned}$$

Hence, by (A.1), we have that

$$\begin{aligned}
&\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}\,\mathfrak{Re}\,\big(\mathcal{R}_{0,\lambda}(\gamma_j\otimes 1)\mathcal{R}_{0,\lambda}\big)\\
&\quad = -(\gamma_j\otimes 1)\mathcal{D}_j\mathcal{D}\int_0^\infty \frac{\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}(1+\lambda+\mathcal{D}^2)^{-2} - \int_0^\infty \frac{(1+\lambda)\,\mathrm{d}\lambda}{\lambda^{\frac{1}{2}}}(1+\lambda+\mathcal{D}^2)^{-2}\\
&\quad = -\frac{\pi}{2}(\gamma_j\otimes 1)\mathcal{D}_j\mathcal{D}(1+\mathcal{D}^2)^{-\frac{3}{2}} - \frac{\pi}{2}(1+\mathcal{D}^2)^{-\frac{3}{2}} - \frac{\pi}{2}(1+\mathcal{D}^2)^{-\frac{1}{2}}.
\end{aligned}$$

Some elementary algebraic manipulation yields the result. □

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