

Trace and index of Dirac–Schrödinger operators on open space with operator potentials

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Abstract. We develop a principal trace and generalized index formula for a Dirac–Schrödinger operator D on open space of odd dimension $d \geq 3$ with a potential given by a family of self-adjoint unbounded operators acting on an infinite-dimensional Hilbert space H . The presented results generalize formulas surrounding the Callias index theorem to the case of unbounded operator potentials, for which the operator D is not necessarily Fredholm. This is the principal novelty of this paper. As application, we include examples where the trace formula is used to calculate the Witten index of non-Fredholm massless $(d + 1)$ -Dirac–Schrödinger operators acting in $L^2(\mathbb{R}^{d+1}, H)$.

1. Introduction

The central goal of this paper is to calculate the trace (called in the following the “principal trace”) $\mathrm{tr}_{L^2(\mathbb{R}^d, H)} \mathrm{tr}_{\mathbb{C}^r} (e^{-tD^*D} - e^{-tDD^*})$, $t > 0$, of the Dirac–Schrödinger operator $D = i\not{D} + A$, and the associated index formula, under suitable conditions on the operator-valued potential A .

Let us start with the setup, explaining the notation above. We fix i as the imaginary unit in $\mathbb{C}$. Let H be a separable complex Hilbert space, and let A_0 be a self-adjoint operator in H with domain $\mathrm{Dom} A_0$, which plays the role of a “model operator”. We equip domains of (Borel) functions f of A_0 with the corresponding graph norm, which turns $\mathrm{Dom} f(A_0)$ into a separable Hilbert space, embedding continuously into H with norm ≤ 1 . Fix $d \in \mathbb{N}$, $d \geq 3$, to be the odd dimension of the euclidean space $\mathbb{R}^d$, and let A be a function on $\mathbb{R}^d$ with values in the self-adjoint operators in H with constant domain $\mathrm{Dom} A(x) = \mathrm{Dom} A_0$, $x \in \mathbb{R}^d$. Denote by M_0 the constant operator function $\mathbb{R}^d \ni x \mapsto A_0$. Fix $r \in \mathbb{N}$ as the rank (the minimal choice is $r = 2^{\frac{d-1}{2}}$) of Clifford matrices $(c^i)_{i=1}^d \subset \mathbb{C}^{r \times r}$; i.e., for $i, j \in \{1, \dots, d\}$,

$$c^i c^j + c^j c^i = -2\delta_{ij} \mathbb{1}_{\mathbb{C}^r}. \quad (1)$$

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For $p \in [1, \infty]$, denote by $L^p(\mathbb{R}^d, \mathbb{C}^r \otimes H)$ the $\mathbb{C}^r \otimes H$ -valued L^p elements, and with slight abuse of notation, denote by A and M_0 the multiplication operators in the Hilbert space $L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)$, given by

$$\begin{aligned}(Af)(x) &:= A(x)f(x), \quad x \in \mathbb{R}^d, \quad f \in \text{Dom } A, \\ (M_0f)(x) &:= A_0f(x), \quad x \in \mathbb{R}^d, \quad f \in \text{Dom } M_0, \\ \text{Dom } A &:= \text{Dom } M_0 := L^2(\mathbb{R}^d, \mathbb{C}^r \otimes \text{Dom } A_0).\end{aligned}$$

Denote by $H^k(\mathbb{R}^d, \mathbb{C}^r \otimes H)$ the L^2 -Sobolev space of order $k \in \mathbb{N}_0$ with values in $\mathbb{C}^r \otimes H$. Let $\not\partial$ be the Dirac operator in $\mathbb{C}^r \otimes H$ given by

$$\begin{aligned}(\not\partial f)(x) &:= \sum_{i=1}^d c^i (\partial_i f)(x), \quad x \in \mathbb{R}^d, \quad f \in \text{Dom } \not\partial, \\ \text{Dom } \not\partial &:= H^1(\mathbb{R}^d, \mathbb{C}^r \otimes H).\end{aligned}$$

It is well known that $\not\partial$ is self-adjoint, with $\Delta = \not\partial^2 = \Delta_{\mathbb{R}^d} \otimes \mathbb{1}_{\mathbb{C}^r \otimes H}$, where $\Delta_{\mathbb{R}^d}$ is the self-adjoint euclidean Laplace operator $\Delta_{\mathbb{R}^d} := -\sum_{i=1}^d \partial_i^2$, $\text{Dom } \Delta_{\mathbb{R}^d} := H^2(\mathbb{R}^d)$. In $L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)$, introduce the operators D , D_0 given by

$$\begin{aligned}D &:= i\not\partial + A, \quad D_0 := i\not\partial + M_0, \\ \text{Dom } D &= \text{Dom } D_0 = \text{Dom } \not\partial \cap \text{Dom } M_0.\end{aligned}$$

D_0 is normal with $D_0^* = -i\not\partial + M_0$, and $\text{Dom } D_0^* = \text{Dom } D_0$ (cf. [24, Lemma 4.2]). We introduce the non-negative operator H_0 given by

$$\begin{aligned}H_0 &:= D_0 D_0^* = D_0^* D_0 = \Delta + M_0^2, \\ \text{Dom } H_0 &= H^2(\mathbb{R}^d, \mathbb{C}^r \otimes H) \cap \text{Dom } M_0^2.\end{aligned}$$

In the following preparatory section, we will give conditions on A , such that the domain conditions

$$\text{Dom } DD^* = \text{Dom } D^*D = \text{Dom } H_0, \quad \text{Dom } D = \text{Dom } D^* = \text{Dom } D_0$$

are satisfied. We will also show that under further assumptions on the function A , akin to the asymptotic homogeneity condition imposed classically in Callias original paper [13, Theorem 2], the partial trace $\text{tr}_{\mathbb{C}^r}(e^{-tD^*D} - e^{-tDD^*})$ is trace-class in $L^2(\mathbb{R}^d, H)$ for $t > 0$. After introducing a suitable approximation of the operator function A , the bulk of this paper then deals with the calculation of the principal trace.

For the purpose of this introduction, let us now present the most important conditions we impose on the operator function $A = B + M_0$ and discuss some of the details. We use the following notation: $\langle x \rangle_z := (|x|^2 + z)^{\frac{1}{2}}$, and $\langle x \rangle := \langle x \rangle_1$.

Hypothesis 1.1 (Conditions (14) and (15) of Hypothesis 2.12¹). Let $\alpha \geq 1$, and $N \geq \lfloor \frac{\alpha-1}{2}(d+1) \rfloor + 1$. Let B be a family of symmetric operators in H , with domains $\text{Dom } A_0$. Assume that $B\langle A_0 \rangle^{-1}$ is continuously differentiable in the strong operator topology, and that for all $\beta \in [-2N-1, 2N+1]$ the operators $\langle A_0 \rangle^\beta B(x) \langle A_0 \rangle^{-1-\beta}$ are closable for all $x \in \mathbb{R}^d$ with bounded closures and

$$\| \overline{\langle M_0 \rangle^\beta B \langle M_0 \rangle^{-1-\beta}} \|_{L^\infty(\mathbb{R}^d, B(H))} < \infty. \quad (2)$$

Assume that, for $\beta = \pm 2N$,

$$\begin{aligned} & \| \langle M_0 \rangle^\beta B \langle M_0 \rangle^{-\beta} \langle M_0 \rangle_z^{-1} \|_{L^\infty(\mathbb{R}^d, B(H))} \\ & + \| \langle M_0 \rangle^{1+\beta} B \langle M_0 \rangle^{-1-\beta} \langle M_0 \rangle_z^{-1} \|_{L^\infty(\mathbb{R}^d, B(H))} \\ & + \| \langle M_0 \rangle^\beta \nabla B \langle M_0 \rangle^{-1-\beta} \langle M_0 \rangle_z^{-1} \|_{L^\infty(\mathbb{R}^d, B(H)^d)} \\ & \xrightarrow{w \rightarrow \infty} 0, \quad w := \text{dist}(z, (-\infty, 0]). \end{aligned} \quad (3)$$

Further, assume that, for all $\beta \in [-2N + \alpha, 2N + 1]$, there exists $\varepsilon > 0$, such that

$$\begin{aligned} & \| x \mapsto \langle x \rangle \langle A_0 \rangle^{-\alpha+\beta} (\nabla B)(x) \langle A_0 \rangle^{-\beta} \|_{L^\infty(\mathbb{R}^d, S^d(H)^d)} \\ & + \| x \mapsto \langle x \rangle^{1+\varepsilon} \langle A_0 \rangle^{-\alpha+\beta} (\partial_R B)(x) \langle A_0 \rangle^{-\beta} \|_{L^\infty(\mathbb{R}^d, S^d(H))} < \infty, \end{aligned} \quad (4)$$

where $\partial_R := \sum_{i=1}^d \frac{x^i}{|x|} \partial_i$ denotes the radial vector field, and $S^d(H)$ the d -th Schatten–von Neumann class of H .

Aside from these crucial conditions, we also impose a number of mild continuity conditions at infinity, which are displayed in the second and third sets of conditions of Hypothesis 2.12. Exemplarily, such a continuity condition is the following: let $S_1(0)$ denote the $(d-1)$ -dimensional unit sphere, and assume that for $\phi \in \text{Dom } A_0$, a.e. $y \in S_1(0)$, and a.e. $x \in \mathbb{R}^d$,

$$\begin{aligned} & \lim_{R \rightarrow \infty} R \| (\nabla B(Ry + x) - \nabla B(Ry)) \phi \|_{H^d} \\ & = \lim_{R \rightarrow \infty} \| (B(Ry + x) - B(Ry)) \phi \|_H = 0. \end{aligned} \quad (5)$$

Let us give an overview over the above conditions. We first note that the parameter $\alpha \geq 1$ is central. It allows flexibility in the most important condition (4) where a larger α means a weaker requirement on B . Because $N \geq \lfloor \frac{\alpha-1}{2}(d+1) \rfloor + 1$, increasing α implies that N needs to be chosen larger. The parameter N determines how regular B needs to be on the Hilbert scale generated by A_0 (cf. conditions (2) and (3)). However, it should be noted that the regularity of B on $\mathbb{R}^d$ must be in any case just once

¹The statements are mathematically the same with expanded notation.

continuously differentiable, regardless of the choice of α , and thus N . Condition (3) encodes Kato–Rellich bounds on the family B , which in particular implies that all $A(x) = B(x) + A_0$ have constant domain $\text{Dom } A_0$. In rough terms, condition (3) ensures that the domain properties of the involved operators are well behaved. Condition (4) stipulates the (relative) Schatten–von Neumann membership of the derivatives of the operator function B and their decay for $|x| \rightarrow \infty$. The radial derivative is singled out, since we assume that it decays faster. These decay conditions correspond to the assumption of asymptotic homogeneity of order 0 in Callias’ classical setup [13, Theorem 2]. The exemplar continuity condition (5) also refers to the behaviour of B at infinity. Roughly speaking, it implies that it should not matter on which ray one approaches a fixed direction at infinity of the functions B and ∇B . The other continuity assumptions we make, which are displayed in the third set of conditions of Hypothesis 2.12, follow the same pattern. We note that these continuity conditions are, for example, satisfied if B is eventually radially constant, i.e., $B(x) = \tilde{B}(\frac{x}{|x|})$ for $|x|$ large enough, and $\tilde{B}$ sufficiently smooth.

It should be remarked that while the above conditions are quite general, one should also emphasize that the possibility of arbitrarily choosing $\alpha \geq 1$ is not only interesting for generality but also because of the requirements from applications. If one wants to incorporate the choice of a proper differential operator of order 1 on $\mathbb{R}^n$ for A_0 itself (H is then $L^2(\mathbb{R}^n)$), one runs into problems with condition (4) if one is just allowed to take $\alpha = 1$. Due to the well-known Schatten–von Neumann estimates (cf. [36, Chapter 4]), this issue boils basically down to the fact that x^{-n} is not integrable on $\mathbb{R}^n$ at infinity. We note that at the end of this paper we include as an example results dealing with exactly this sketched setup, which come from [23], which gives the detailed proofs in this particular setup, which we omit in this paper.

After explaining the conditions imposed on the operator potential A , let us present the main result of this paper, which is the desired principal trace formula in terms of A and dA in a neighbourhood of infinity.

Theorem 1.2 (Theorem 6.4). *Assume Hypothesis 2.12. For $\phi \in C_c^\infty(\mathbb{R}^d)$, denote $A_\phi := A_0 + (1 - \phi)(A - A_0)$. Then, for $t > 0$, and any $\phi \in C_c^\infty(\mathbb{R}^d)$,*

$$\begin{aligned} & \text{tr}_{L^2(\mathbb{R}^d, H)} \text{tr}_{C^r} (e^{-tD^*D} - e^{-tDD^*}) \\ &= \frac{2}{d} (4\pi)^{-\frac{d}{2}} i^d \kappa_c t^{\frac{d}{2}} \int_{s \in \Delta_{d-1}} \int_{\mathbb{R}^d} \text{tr}_H \bigwedge_{j=0}^{d-1} (dA_\phi e^{-ts_j A_\phi^2}) ds, \end{aligned} \quad (6)$$

where (6) is independent of the choice of ϕ , and

$$\kappa_c := \text{tr}_{C^r} (c^1 \cdot \dots \cdot c^d),$$

$\Delta_{d-1} = \{u \in [0, 1]^d, \sum_{j=0}^{d-1} u_j = 1\}$ denotes the $(d-1)$ -simplex, and $\bigwedge$ the exterior product.

We note that formula (6) only depends on the values of A and dA in a neighbourhood of infinity due to the cut-off ϕ . If A and dA additionally assume radial limits in a particular sense, we show that only these limits appear in the trace formula.

Corollary 1.3 (Corollary 6.5). *Assume Hypothesis 2.12, and denote*

$$A^\circ(y)\psi := \lim_{R \rightarrow \infty} A(Ry)\psi,$$

for $\psi \in \text{Dom } A_0$, and $y \in S_1(0)$. Assume that $A^\circ\psi$ is differentiable on $S_1(0)$ for $\psi \in \text{Dom } A_0$, such that for a.e. $y \in S_1(0)$,

$$\lim_{R \rightarrow \infty} R \|\partial_i A^\circ(y)\psi - \partial_i A(Ry)\psi\|_H = 0,$$

and that for $\beta \in [-2N + \alpha, 2N + 1]$, and all unit vector fields v in $TS_1(0)$,

$$\langle A_0 \rangle^{-\alpha+\beta} (vA^\circ) \langle A_0 \rangle^{-\beta} \in L^\infty(S_1(0), S^d(H)).$$

Denote, for $\rho \in C_c^\infty(\mathbb{R})$,

$$\widetilde{A}_\rho^\circ(x) := A_0 + (1 - \rho(|x|)) \left(A^\circ \left(\frac{x}{|x|} \right) - A_0 \right).$$

Then, for $t > 0$, and any $\rho \in C_c^\infty(\mathbb{R})$, with $\rho \equiv 1$ near 0,

$$\begin{aligned} & \text{tr}_{L^2(\mathbb{R}^d, H)} \text{tr}_{\mathbb{C}^r} (e^{-tD^*D} - e^{-tDD^*}) \\ &= \frac{2}{d} (4\pi)^{-\frac{d}{2}} i^d \kappa_c t^{\frac{d}{2}} \int_{s \in \Delta_{d-1}} \int_{\mathbb{R}^d} \text{tr}_H \bigwedge_{j=0}^{d-1} ((d\widetilde{A}_\rho^\circ) e^{-ts_j \widetilde{A}_\rho^{\circ 2}}) du, \end{aligned}$$

independent of the choice of ρ .

As a direct application of the principal trace formula of Theorem 1.2, we may calculate the Fredholm index of D , whenever D is Fredholm.

Theorem 1.4 (Theorem 7.3). *Assume Hypothesis 2.12. Assume that there exists $R_0 \geq 0$, such that, for $|x| \geq R_0$, we have $0 \in \rho(A(x))$. Then, D is Fredholm, and the Fredholm index $\text{ind } D$ is given by*

$$\text{ind } D = \frac{2}{d} (4\pi)^{-\frac{d}{2}} i^d \kappa_c \lim_{t \rightarrow \infty} t^{\frac{d}{2}} \int_{s \in \Delta_{d-1}} \int_{\mathbb{R}^d} \text{tr}_H \bigwedge_{j=0}^{d-1} ((dA_\phi) e^{-ts_j A_\phi^2}) ds, \quad (7)$$

where $A_\phi := A_0 + (1 - \phi)(A - A_0)$ for any $\phi \in C_c^\infty(\mathbb{R}^d)$. Formula (7) is independent of the choice of ϕ .

The principal trace formula of Theorem 1.2 can also be applied to determine some cases of a generalized version of index, the so-called (partial) Witten index, of the operator D . The notion was introduced in [26]. We give here the definition of the semi-group regularized partial Witten index.

Definition 1.5. Let T be a linear, densely defined operator $\mathbb{C}^r \otimes X$ for some separable complex Hilbert space X . We say the partial (semi-group regularized) Witten index of T exists, if for some $t_0 > 0$, we have

$$\mathrm{tr}_{\mathbb{C}^r} (e^{-tT^*T} - e^{-tTT^*}) \in S^1(X), \quad t \geq t_0,$$

and if the limit

$$\mathrm{ind}_W T := \lim_{t \rightarrow \infty} \mathrm{tr}_X (\mathrm{tr}_{\mathbb{C}^r} (e^{-tT^*T} - e^{-tTT^*}))$$

exists, then $\mathrm{ind}_W T$ is called the partial Witten index of T .

The (partial) Witten index may assume any real number (cf. [7, 14, 16] in dimension $d = 1$, and [23] for $d \geq 3$); however, if T is additionally Fredholm, it coincides with the usual Fredholm index (see Remark 7.2).

We conclude this paper, as we mentioned before, with examples of partial Witten index formulas taken from [23] without their proofs, dealing with massless $(d + 1)$ -Dirac–Schrödinger operators. These operators are non-Fredholm, but possess partial Witten index formulas given in Example 7.5, and for a special choice of potential in Example 7.7. The point of these examples is that they extend the known Witten index formula, given directly in terms of the underlying potential, in the case $d = 1$ (cf. [7, 14, 16]), to $d \geq 3$ odd. In this presented setup, the model operator $A_0 = i\partial$ is just the derivative in one direction, and B is given by a (matrix) potential over $\mathbb{R}^{d+1}$.

Definition 1.6. For a potential $V : \mathbb{R}^d \times \mathbb{R} \rightarrow B_{sa}(H)$, define the associated *massless* $(d + 1)$ -Dirac–Schrödinger operator D_V ,

$$(D_V f)(x, y) := i \sum_{j=1}^d c^j \partial_{x^j} f(x, y) + i \partial_y f(x, y) + V(x, y) f(x, y),$$

$$x \in \mathbb{R}^d, \quad y \in \mathbb{R}, \quad f \in W^{1,2}(\mathbb{R}^{d+1}, \mathbb{C}^r \otimes H).$$

Without going into the details of the assumptions on the potential V , we then have the index formula.

Example 1.7 (Example 7.5). Assume that V satisfies the requirements given in Example 7.5. Then,

$$\mathrm{ind}_W D_V = \frac{1}{2\pi} (4\pi)^{-\frac{d-1}{2}} \frac{(\frac{d-1}{2})!}{d!} \kappa_c \int_{\mathbb{R}^d} \mathrm{tr}_H ((U^V)^{-1} dU^V)^{\wedge d},$$

where $\wedge^d$ is the d -fold exterior power,

$$\kappa_c := \operatorname{tr}_{\mathbb{C}^r} (c^1 \cdot \dots \cdot c^d),$$

and the unitary U^V is given by $U^V(x) := \lim_{n \rightarrow \infty} U^{V(x, \cdot)}(n, -n)$, $x \in \mathbb{R}^d$, where $U^A(y_1, y_2)$, $y_1, y_2 \in \mathbb{R}$, for a given $A : \mathbb{R} \rightarrow B_{sa}(H)$ is the (unique) evolution system of the equation

$$u'(y) = iA(y)u(y), \quad y \in \mathbb{R}.$$

At the end of this introduction, we will compare our results with the existing literature and the history of the problem, but before we do that, let us heuristically summarize the idea of proof of the central Theorem 1.2.

Apart from introducing the main Hypothesis 2.12 in Section 2, the goal of this section is to show domain stability under perturbation induced by the operator family B and then prove a uniform trace-class norm estimate on the partial trace of the resolvent difference of the operators D^*D and DD^* . The core result here is Proposition 2.28, which decomposes the mentioned resolvent difference into a finite sum of products of operators which are either bounded or of appropriate Schatten–von Neumann class. The uniformity in the resolvent parameter allows us to apply holomorphic functional calculus to also obtain the trace-norm estimate for the semi-group difference of D^*D and DD^* in Proposition 2.29.

In Section 3, we then develop an iterative approximation scheme $B_{n,m,l}$ for the operator family B , such that the resulting trace formulae will converge. The main result in this section is Corollary 3.4. The reason for this procedure is to improve the properties of B ; essentially, we show that without loss of generality one may assume that B is smooth and finite rank valued. This, in particular, enables us in the subsequent sections to use the commutation under the trace more freely.

Section 4 then develops the overarching framework to calculate the trace as the integral over the diagonal of the fibre trace of an appropriate operator-valued integral kernel. This is a classical technique in the matrix valued case but requires some justification in our setup. The operator valued integral kernels we need are then constructed as perturbations of the Gaussian heat kernel by a Volterra-series-type argument, which is again a classical approach in the matrix valued case. For the idea of proof, we should highlight Lemma 4.8, which decomposes the semi-group difference into a finite sum of integrals of commutators. There are two types of commutators, those with $[i\partial, \bullet]$ and those with $[A, \bullet]$. We will later show that the commutator with the multiplication by A will vanish in the fibre trace of its integral kernel diagonal as expected, while the trace of the commutator with $i\partial$ will allow us to use Stokes' theorem to pass to integrals over expanding spheres $S_R(0)$, $R \rightarrow \infty$, similar to Callias' classical result.

In Section 5, this procedure is carried out with the appropriate integral kernels constructed from the auxiliary integral kernels in Section 4. We then exploit, as mentioned

before, that only the values of the involved integral kernels on the spheres $S_R(0)$ for $R \rightarrow \infty$ matter, and only those expressions which do not decay faster than $R^{d-1} \sim \text{vol}(S_R(0))$ survive. The main result of this section is, therefore, Proposition 5.9, a preliminary trace formula involving the values of a particular integral kernel $\kappa_s^{-,d-1}(x, x)$ for $x \in S_R(0)$.

The next step of the proof is provided in Section 6, where we show first that the particular kernel $\kappa_s^{-,d-1}$ can be replaced successively by increasingly more tractable integral kernels in the spherical limit on $S_R(0)$, $R \rightarrow \infty$, which is the content of Lemma 6.3, the last step before the main result, namely, Theorem 6.4. In its proof, the essential step is to pass to the limits of the approximation of B , which was introduced in Section 3.

Before we proceed, let us outline the historical context of the problem. A differential operator of the type $D = i\partial + A$ was discussed prominently by Atiyah, Patodi, and Singer in their seminal series of papers [3–5]. Therein, A is a family over $\mathbb{R}$ of first-order, elliptic, differential operators on a compact, odd-dimensional manifold with invertible asymptotic endpoints. They showed that D is Fredholm with Fredholm index $\text{ind } D = \text{sflow}(A, 0)$, where the right-hand side is the spectral flow of A through 0. The one-dimensional case, in which A is parametrized over $\mathbb{R}$, and $i\partial$ is just the derivative along $\mathbb{R}$, was further discussed by Robbin and Salamon [33] for more general types of unbounded operator families A , however still with $A(x)$, $x \in \mathbb{R}$, having discrete spectra. One should also note [7], where some of the notions about generalized index, and spectral flow, appeared. In 2008, Pushnitski showed in [31] that discreteness of the spectrum of A can, in essence, be replaced by the following assumption: assume that $A = A_- + B$, where A_- is a generic self-adjoint operator in a separable Hilbert space, and the derivative B' of the family B of bounded, symmetric operators is an integrable family of trace-class operators in H , i.e.,

$$\int_{\mathbb{R}} \|B'(x)\|_{S^1(H)} < \infty. \quad (8)$$

Under these conditions, D is Fredholm with

$$\text{ind } D = \xi(0, A_+, A_-),$$

where $A_{\pm} = \lim_{x \rightarrow \pm\infty} A(x)$ are the (self-adjoint) limit endpoints in a certain sense, and $\xi(\cdot, A_+, A_-)$ is the associated spectral shift function, a concept from scattering theory (cf. [39]) which we will not delve into here; however, it should be noted that if the spectral shift function of the endpoints and the spectral flow of a (regular enough) family exist, then they coincide (cf. also [7]). However, Pushnitski's results go beyond a generalization of the index problem. In fact, a principal trace formula (which in general carries more information on D than the Fredholm index), already present in

Callias paper [13], was shown in this more general setup:

$$\begin{aligned} \operatorname{tr}_{L^2(\mathbb{R}, H)}((DD^* - z)^{-1} - (D^*D - z)^{-1}) \\ = \frac{1}{2z} \operatorname{tr}_H(A_+(A_+^2 - z)^{-\frac{1}{2}} - A_-(A_-^2 - z)^{-\frac{1}{2}}) \end{aligned} \quad (9)$$

for $z \in \mathbb{C} \setminus [0, \infty)$. In the following years, and also quite recently, more results emerged similar to Pushnitski's trace-based approach to the index problem; for example, condition (8) was replaced with

$$\int_{\mathbb{R}} \|B'(x)(A_-^2 + 1)^{-\frac{1}{2}}\|_{S^1(H)} < \infty,$$

by Gesztesy et al., in [24], while (9) still holds. Further generalizations along these lines have been discussed in [15, 17]. These results are presented comprehensively in the monograph [18]. We remark that the principal trace formula in these publications (9) corresponds to the case $d = 1$ in the principal trace formula (6) presented in this paper, if one rewrites the right-hand side of (9) with an appropriate integral (the endpoints $A_{\pm}$ can be seen as the endpoints of the function $A(t) = A_- + t(A_+ - A_-)$, an application of the fundamental theorem of calculus then yields the integrated form), and turned via the inverse Laplace transform into an exponentiated version instead of the resolvent version (9):

$$\operatorname{tr}_{L^2(\mathbb{R}, H)}(e^{-tD^*D} - e^{-tDD^*}) = \sqrt{\frac{t}{\pi}} \int_0^1 \operatorname{tr}_H(e^{-tA(s)^2}(A_+ - A_-)) ds.$$

Another important result, extending the classical "Index=Spectral Flow" Theorem, was provided by Callias in the paper [13]. While the operator family A acts there in a finite-dimensional space, the index formula therein holds for $\not{D}$ being the classical Dirac operator in $\mathbb{R}^d$ for d odd, which is also our setup here. The index theorem [13, Theorem 2] then reads as follows: let $k = \frac{d-1}{2}$. With the minimal rank choice $r = 2^k$ for the Clifford matrices, let A be a smooth family of $m \times m$ -matrices with $|A(x)| \geq C > 0$ for all $|x| \geq c$ for some constants c, C . Assume that A is asymptotically homogeneous of order 0 as $x \rightarrow \infty$ (i.e., $A(x)$ is a 0-order classic symbol in x). Then, D is Fredholm, and, with $U(x) := A(x)|A(x)|^{-1}$,

$$\operatorname{ind} D = \frac{1}{2k!} \left(\frac{i}{8\pi} \right)^k \lim_{R \rightarrow \infty} \int_{S_R} \operatorname{tr}_{C^m} U(dU)^{\wedge(d-1)}, \quad (10)$$

here, S_R denotes the $d - 1$ -sphere of radius R around 0, and $(dU)^{\wedge(d-1)}$ the $d - 1$ -fold exterior product of (matrix-)one-forms dU . One should note that there are some problems with the trace-class membership of certain operators in [13] in the original

proof;² however, the ideas have been made rigorous (and generalized) by Gesztesy and Waurick in [27].

Despite being beyond the scope of this paper, one should also mention that there exist a multitude of generalizations of Callias' index theorem to non-compact Riemannian manifolds (cf. [1, 2, 9, 10, 12, 19, 20, 29, 30, 32, 34, 35, 37, 38]), however still in the context of Fredholmness and not providing a general principal trace formula. The usual assumption therein is that the operator valued potential A is invertible in some sense outside a compact region of the manifold to ensure Fredholmness of D . We emphasize that we do not assume such a condition in this paper.

With this perspective, the principal trace formula (6) stands in analogy to (10), similar in spirit to the generalizations developed by Pushnitski in the one-dimensional case for the "Index=Spectral Flow"-Theorem, especially if one no longer requires D to be Fredholm.

2. Trace-class properties of the resolvents of D^*D and DD^*

In this section, we present our conditions on the family A and show domain and trace-class properties. We start, however, by introducing further notation.

Denote by $S^p(H)$ the p -th Schatten–von Neumann class of H , and by $B(H)$ the linear bounded operators of H . Denote $\langle T \rangle_z := (T^*T + z)^{\frac{1}{2}}$, $z \in \mathbb{C} \setminus (-\infty, 0]$, and $\langle T \rangle := \langle T \rangle_1$, for an operator T in a Hilbert space. Denote for a measurable function $g : \mathbb{R} \rightarrow \mathbb{R}$ by $g(X)$ the multiplication operator in $L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)$, given by $(g(X)f)(x) := g(x)f(x)$, $x \in \mathbb{R}^d$. For $z \in \rho(T)$, denote $R_z(T) := (T + z)^{-1}$.

The following simple relation between trace and Clifford matrices is essential.

Lemma 2.1. (1) For $n \in \mathbb{N}$ and $\alpha \in \{1, \dots, d\}^n$,

$$\mathrm{tr}_{\mathbb{C}^r} \left(\prod_{j=1}^n c^{\alpha_j} \right) = 0,$$

if (n, d) are odd, and $n < d$ or $(n$ is odd, and d is even).

(2) For d odd, and $\alpha \in \{1, \dots, d\}^d$,

$$\mathrm{tr}_{\mathbb{C}^r} \left(\prod_{j=1}^d c^{\alpha_j} \right) = \kappa_c \varepsilon_\alpha, \quad (11)$$

²This may be due to the fact that shortly after Callias published his results a different proof was presented by Bott and Seeley in [8], which Callias already mentions in the introduction of his paper.

where $\varepsilon_\alpha = \varepsilon_{\alpha_1 \dots \alpha_d}$ is the Levi-Civita symbol, and

$$\kappa_c := \operatorname{tr}_{\mathbb{C}^r} \left(\prod_{j=1}^d c^j \right).$$

If $r = 2^{\frac{d-1}{2}}$, i.e., the minimal choice of r to satisfy the anti-commutator relation (1), then

$$\kappa_c = (2i)^{\frac{d-1}{2}} l(-i)^d.$$

Proof. Due to the anti-commutator relation (1), it is sufficient to consider only those α , for which all α_j , $j \in \{1, \dots, n\}$, are pairwise different. Since n is odd, we have $n < d$ in any case. Thus, there exists $m \in \{1, \dots, d\}$ such that $m \neq \alpha_j$, $j \in \{1, \dots, n\}$. Then,

$$\begin{aligned} \operatorname{tr}_{\mathbb{C}^r} \left(\prod_{j=1}^n c^{\alpha_j} \right) &= -\operatorname{tr}_{\mathbb{C}^r} \left((c^m)^2 \prod_{j=1}^n c^{\alpha_j} \right) \\ &= -\operatorname{tr}_{\mathbb{C}^r} \left(c^m \prod_{j=1}^n c^{\alpha_j} c^m \right) = (-1)^{n+1} \operatorname{tr}_{\mathbb{C}^r} \left((c^m)^2 \prod_{j=1}^n c^{\alpha_j} \right) \\ &= -\operatorname{tr}_{\mathbb{C}^r} \left(\prod_{j=1}^n c^{\alpha_j} \right). \end{aligned}$$

Statement (11) follows immediately from the anti-commutator relation (1), the definition of ε_α , and the first part of this proof. The case of $r = 2^{\frac{d-1}{2}}$ follows by induction in d and the representation of Clifford matrices of odd dimension d by those of dimension $d - 2$. The sign convention corresponds to the choice $c^j = -i\sigma^j$, where σ^j are the classical Pauli matrices. ■

Definition 2.2. For B an function on $\mathbb{R}^d$ with values in symmetric operators in H with common domain $\operatorname{Dom} A_0$, let $D = D_B := i\rlap{-}\not{D} + B + M_0$, $\operatorname{Dom} D_B := \operatorname{Dom} D_0$, and $H_B := \Delta + (B + M_0)^2$, $\operatorname{Dom} H_B := \operatorname{Dom} H_0$.

Definition 2.3. For B a operator function on $\mathbb{R}^d$ with domains $\operatorname{Dom} B(x) = \operatorname{Dom} A_0$, we write $B \in C_b^k(\mathbb{R}^d, A_0, m)$, for $k \in \mathbb{N}_0$, $m \geq 0$, if $\langle A_0 \rangle^\beta B(x) \langle A_0 \rangle^{-1-\beta}$, $x \in \mathbb{R}^d$, is a family of closable operators with closures in $B(H)$ for any $\beta \in [-m, m]$, and $x \mapsto \overline{\langle A_0 \rangle^\beta B(x) \langle A_0 \rangle^{-1-\beta}} \in C_b^k(\mathbb{R}^d, B(H))$, where C_b^k is the space of k -times continuously differentiable bounded functions in the strong operator topology with bounded derivatives, where boundedness is with respect to the $B(H)$ operator norm. As usual, $C_b^k(\mathbb{R}^d)$ just denotes the scalar/matrix valued- C_b^k -functions. All involved spaces come equipped with the obvious norm given by summing the appropriate L^∞ -norms of the derivatives up to order k .

Definition 2.4. We introduce the following semi-norms for operators

$$B \in C_b^1(\mathbb{R}^d, A_0, 1),$$

with $z \in \mathbb{C} \setminus (-\infty, 0]$,

$$\begin{aligned} \rho_z(B) := & \|B \langle M_0 \rangle_z^{-1}\|_{L^\infty(\mathbb{R}^d, B(H))} + \|\langle M_0 \rangle B \langle M_0 \rangle^{-1} \langle M_0 \rangle_z^{-1}\|_{L^\infty(\mathbb{R}^d, B(H))} \\ & + \|\nabla B \langle M_0 \rangle^{-1} \langle M_0 \rangle_z^{-1}\|_{L^\infty(\mathbb{R}^d, B(H)^d)}. \end{aligned}$$

For $\beta \in \mathbb{R}$, denote, for $B \in C_b^1(\mathbb{R}^d, A_0, |\beta| + 1)$,

$$\rho_z^\beta(B) := \rho_z(\langle M_0 \rangle^\beta B \langle M_0 \rangle^{-\beta}).$$

Remark 2.5. Complex interpolation implies certain operator inequalities (cf. [25]). In particular, by combining [25, Theorem 2.8] with Jensen's inequality, we have, for $\beta \in [-2N, 2N]$,

$$\rho_z^\beta(B) \leq \rho_z^{-2N}(B) + \rho_z^{2N}(B).$$

Proposition 2.6. Let a family $B \in C_b^1(\mathbb{R}^d, A_0, 1)$ of symmetric operators satisfy

$$\lim_{\text{dist}(z, (-\infty, 0]) \rightarrow \infty} \rho_z(B) = 0. \quad (12)$$

Then, D_B is closed in $L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)$ with $D_B^* = -i\rlap{/}\partial + B + M_0$, $\text{Dom } D_B^* = \text{Dom } D_0$. Moreover, the operators $D_B D_B^*$, $D_B^* D_B$, and H_B are non-negative and self-adjoint with domain $\text{Dom } H_0$.

Proof. The proof of the statement about D_B and D_B^* is similar to the proof of [24, Lemma 4.4], although it is assumed that $d = 1$, the argument works with the necessary changes for all dimensions $d \in \mathbb{N}$. Let us provide at least an outline. The authors show that B is relatively bounded by D_0 , and B^* by D_0^* , with bound 0, provided that

$$\|B \langle M_0 \rangle_z^{-1}\|_{L^\infty(\mathbb{R}^d, B(H))} \xrightarrow{\mathbb{R} \ni z \rightarrow \infty} 0.$$

This condition is, however, satisfied by (12). The statement then follows from the Kato–Rellich theorems [28, Theorems 4.1.1, 5.4.3]. The same idea works for $D_B^* D_B$ and $D_B D_B^*$, which are self-adjoint by definition. Let us consider $D_B D_B^*$; the proof for $D_B^* D_B$ is analogous. As differential operators, we have

$$D_B D_B^* = \Delta + (B + M_0)^2 + i(\rlap{/}\partial B),$$

which implies

$$D_B D_B^* - H_0 = B^2 + M_0 B + B M_0 + i(\rlap{/}\partial B)$$

on $\text{Dom } H_0$. We estimate, for $z \geq 1$,

$$\begin{aligned} & \| (B^2 + M_0 B + B M_0 + i\beta^E B) R_{z^2}(H_0) \|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))} \\ & \leq (\|B \langle M_0 \rangle^{-1}\|_{L^\infty(\mathbb{R}^d, B(H))} + 1) \| \langle M_0 \rangle B \langle M_0 \rangle^{-1} \langle M_0 \rangle_z^{-1} \|_{L^\infty(\mathbb{R}^d, B(H))} \\ & \quad + \|B \langle M_0 \rangle_z^{-1}\|_{L^\infty(\mathbb{R}^d, B(H))} \\ & \quad + \|\nabla B \langle M_0 \rangle^{-1} \langle M_0 \rangle_z^{-1}\|_{L^\infty(\mathbb{R}^d, B(H)^d)} \xrightarrow[z \rightarrow \infty]{(12)} 0. \end{aligned}$$

Hence, $(B + M_0)^2 + i(\beta^E B)$ is relatively bounded by H_0 with bound 0. Thus, $D_B D_B^*$ is self-adjoint on $\text{Dom } H_0$, and essentially self-adjoint on any core of H_0 . Since $C_c^\infty(\mathbb{R}^d) \otimes \mathbb{C}^r \otimes \mathcal{D}$ is a common core of both $D_B D_B^*$ and H_0 , we have

$$\text{Dom}(D_B D_B^*) = \text{Dom } H_0.$$

For H_B , we have a similar result, but we have to add that $H_B \geq 0$ on $\text{Dom } H_0$ follows by a direct calculation. ■

Remark 2.7. Under the prerequisites of Proposition 2.6, it also follows that $A(x) = A_0 + B(x)$ is self-adjoint on $\text{Dom } A_0$ for a.e. $x \in \mathbb{R}^d$. Indeed, since $\langle M_0 \rangle_z \langle D_0 \rangle_z^{-1}$ is bounded in norm by 1, uniformly for $z > 0$, it follows from $\|T\|_{B(L^2(\mathbb{R}^d, H))} = \|T\|_{L^\infty(\mathbb{R}^d, B(H))}$ for measurable multiplication operators T that

$$\lim_{z \rightarrow \infty} \sup_{x \in \mathbb{R}^d} \|B(x) \langle A_0 \rangle_z^{-1}\|_{B(H)} = 0,$$

which implies that for a.e. $x \in \mathbb{R}^d$, and $\phi \in \text{Dom } A_0$,

$$\begin{aligned} \|B(x)\phi\|_H &= \|B(x) \langle A_0 \rangle_z^{-1} \langle A_0 \rangle_z (A_0 + i\sqrt{z})^{-1} (A_0 + i\sqrt{z})\phi\|_H \\ &\leq o(1) \|(A_0 + i\sqrt{z})\phi\|_H \leq o(1) \|A_0 \phi\|_H + o(\sqrt{z}) \|\phi\|_H, \quad z \rightarrow \infty. \end{aligned}$$

Hence, $B(x)$ is relatively bounded by A_0 with bound 0 for a.e. $x \in \mathbb{R}^d$. Since $B(x)$ is symmetric, the statement follows from the Kato–Rellich theorem.

Next, we recall some well-known facts about Schatten–von Neumann operators. Let $S^p(X)$ denote the Banach space of the p Schatten–von Neumann operators of a separable Hilbert space X .

Lemma 2.8. *Let $2 \leq p < \infty$, $x \mapsto T(x) \in L^p(\mathbb{R}^d, S^p(\mathbb{C}^r \otimes H))$, and $g \in L^p(\mathbb{R}^d)$; then, $Tg(|\beta|) \in S^p(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ with*

$$\|Tg(|\beta|)\|_{S^p(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))} \leq (2\pi)^{-\frac{d}{p}} \|T\|_{L^p(\mathbb{R}^d, S^p(\mathbb{C}^r \otimes H))} \|g\|_{L^p(\mathbb{R}^d)}. \quad (13)$$

Proof. The proof of this statement is analogous to the proof of [36, Theorem 4.1]. There, $H = \mathbb{C}$, which one has to change here. We give the essential outline. For $p = 2$,

the statement follows from the fact that there is a $L^2(\mathbb{R}^d \times \mathbb{R}^d, S^2(\mathbb{C}^r \otimes H))$ -valued integral kernel k of $Tg(|\not\partial|)$, given by

$$k(x, y) = (2\pi)^{-\frac{d}{2}} T(x) \check{g}(x - y), \quad x, y \in \mathbb{R}^d,$$

where $\check{g}(u) := (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} e^{-iu \cdot \xi} g(\xi) \otimes \mathbb{1}_{\mathbb{C}^r} d\xi$. The operator $Tg(|\not\partial|)$ is, thus, Hilbert–Schmidt with equality in (13). On the other hand, $x \mapsto T(x) \in L^\infty(\mathbb{R}^d, B(\mathbb{C}^r \otimes H))$ implies that $T \in B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$, and Borel functional calculus implies $g(|\not\partial|) \in B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$. We have

$$\|Tg(|\not\partial|)\|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))} \leq \|T\|_{L^\infty(\mathbb{R}^d, B(\mathbb{C}^r \otimes H))} \|g\|_{L^\infty(\mathbb{R}^d)}.$$

If T and g are compactly supported, the case $p \geq 2$ with (13) follows from complex interpolation. For general T and g , let $(\phi_n)_{n \in \mathbb{N}}$ be a sequence of compactly supported continuous functions, which converge pointwise to 1 on $\mathbb{R}$. Then, the self-adjoint operators $\phi_n \otimes \mathbb{1}_{\mathbb{C}^r \otimes H}$ and $\phi_n(|\not\partial|)$ converge strongly to $\mathbb{1}_{L^2(E \otimes H)}$. With $T_n(x) := \phi_n(x)T(x)$ and $g_n := \phi_n g$, we obtain $T_n g_n(|\not\partial|) = \phi_n \otimes \mathbb{1}_{\mathbb{C}^r \otimes H} Tg(|\not\partial|) \phi_n(|\not\partial|)$. By Lemma 2.19 and since $\lim_{n \rightarrow \infty} T_n = T$ in $L^p(\mathbb{R}^d, S^p(\mathbb{C}^r \otimes H))$, and $\lim_{n \rightarrow \infty} g_n = g$ in $L^p(\mathbb{R}^d)$, the general case follows, by taking the limits past the norms in (13). ■

Corollary 2.9. *Let $x \mapsto T(x) \in L^p(\mathbb{R}^d, S^d(\mathbb{C}^r \otimes H))$, such that $T(x)$ is self-adjoint for a.e. $x \in \mathbb{R}^d$. Then, for $t > \frac{d}{p}$, we have a constant $C_{d,p} < \infty$, such that*

$$\begin{aligned} \langle \not\partial \rangle^{s-t} T \langle \not\partial \rangle^{-s} &\in S^p(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)), \\ \|\langle \not\partial \rangle^{s-t} T \langle \not\partial \rangle^{-s}\|_{S^p(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))} &\leq C_{d,p} \|T\|_{L^p(\mathbb{R}^d, S^p(\mathbb{C}^r \otimes H))}, \quad s \in [0, t]. \end{aligned}$$

Proof. First, consider $s = t$. We note that $\xi \mapsto \langle \xi \rangle^{-t} \in L^p(\mathbb{R}^d)$, so Lemma 2.8 applies. The case $s = 0$ follows by taking adjoints. The general case follows by complex interpolation (cf. [25]). ■

Definition 2.10. We introduce a second set of semi-norms for $B \in C_b^1(\mathbb{R}^d, A_0, m)$ (see Definition 2.3), $m \geq 0$, and the following data: $\alpha \geq 0$, $\beta \in \mathbb{R}$, with $|\beta - 1| \leq m$, $|\beta - \alpha| \leq m$, $p \geq 2$, $s \geq 0$, and a unit vector field $v \in \Gamma(T\mathbb{R}^d)$,

$$\tau^{\alpha, \beta, v, p, s}(B) := \|x \mapsto \langle x \rangle^s \langle A_0 \rangle^{-\alpha + \beta} (vB)(x) \langle A_0 \rangle^{-\beta}\|_{L^\infty(\mathbb{R}^d, S^p(H))},$$

and denote

$$\tau^{\alpha, \beta, \nabla, p, s} := \sum_{i=1}^d \tau^{\alpha, \beta, \partial_i, p, s}.$$

To formulate the continuity conditions at infinity, we introduce the following notation.

Definition 2.11. For $x, y \in \mathbb{R}^d$ and an operator-valued function S over $\mathbb{R}^d$, define

$$\begin{aligned}(T_y S)(x) &:= S(x - y), \\ \delta_y &:= T_{-y} - T_y, \\ w_y^2(S) &:= \delta_{\frac{y}{2}}^2 S.\end{aligned}$$

We introduce the set of conditions on the operator family $A = M_0 + B$.

Hypothesis 2.12. Let $\alpha \geq 1$, and $N \geq \lfloor \frac{\alpha-1}{2}(d+1) \rfloor + 1$. Let B be a family of symmetric operators in H , with domains $\text{Dom } A_0$. Assume that $B \in C_b^1(\mathbb{R}^d, A_0, 2N+1)$. Assume that

(1) The operator family B satisfies

$$\lim_{\text{dist}(z, (-\infty, 0]) \rightarrow \infty} \rho_z^{-2N}(B) + \rho_z^{2N}(B) = 0, \quad (14)$$

and that for all $\beta \in [-2N + \alpha, 2N + 1]$,

$$\begin{aligned}\tau^{\alpha, \beta, \nabla, d, 1}(B) &< \infty, \\ \exists \varepsilon > 0 : \tau^{\alpha, \beta, \partial_R, d, 1+\varepsilon}(B) &< \infty,\end{aligned} \quad (15)$$

where $\partial_R := \sum_{i=1}^d \frac{x^i}{|x|} \partial_i$ denotes the radial vector field.

(2) Let $S_1(0)$ denote the $(d-1)$ -dimensional unit sphere. For $\phi \in \text{Dom } A_0$, a.e. $y \in S_1(0)$, a.e. $x \in \mathbb{R}^d$, and $\gamma \in \mathbb{N}_0^d$ with $|\gamma| \leq 1$, assume that

$$\lim_{R \rightarrow \infty} R^{|\gamma|} \|(\partial^\gamma B(Ry + x) - \partial^\gamma B(Ry))\phi\|_H = 0. \quad (16)$$

(3) Assume that in case $d = 3$ there exists $\delta > 0$ such that for a.e. $y \in S_1(0)$, $z' \in \mathbb{R}^d$, for $\phi \in \text{Dom } A_0^2$, and $c > 0$,

$$\begin{aligned}\sup_{|x| \geq 1} |x|^{\frac{1}{2}} \sup_{z \in B_{c \log |x|}(0)} \|(B(x+z) - B(x))\phi\|_H &< \infty, \\ \sup_{|x| \geq 1} |x| \sup_{z \in B_{c \log |x|}(0)} \|w_z^2(B)(x)\phi\|_H &< \infty, \\ \sup_{|x| \geq 1} |x|^{\frac{3}{2}} \sup_{z \in B_{c \log |x|}(0)} m_d(z) \|(\nabla B(x+z) - \nabla B(x))\phi\|_H &< \infty, \\ \sup_{|x| \geq 1} |x|^2 \sup_{z \in B_{c \log |x|}(0)} m_d(z) \|w_z^2(\nabla B)(x)\phi\|_H &< \infty, \\ \lim_{R \rightarrow \infty} R \|w_{z'}^2(B)(Ry)\phi\|_H &= 0, \\ \lim_{R \rightarrow \infty} R^2 \|w_{z'}^2(\nabla B)(Ry)\phi\|_H &= 0,\end{aligned}$$

where

$$m_d(z) := \begin{cases} \min(1, |z|)^{-\delta}, & d = 3, \\ 1, & d \geq 5. \end{cases}$$

Remark 2.13. By a Kato–Rellich argument, Hypothesis 2.12 implies that, for a.e. $x_0 \in \mathbb{R}^d$, $A(x_0) = A_0 + B(x_0)$ can take the role of the model operator A_0 .

The second and third sets of conditions concerned with the radial convergence at infinity of A and dA will also only play a role in determining the trace. Note that the prerequisites of Proposition 2.6 and Remark 2.7 are satisfied if B satisfies Hypothesis 2.12.

In the following, we will prepare for the proof of Proposition 2.28. In this proof, we will factorize the partial trace of difference of the resolvent powers of DD^* and D^*D into appropriate bounded and Schatten–von Neumann class operators. These factors will fit the templates of operators we will discuss below.

Definition 2.14. Let B satisfy Hypothesis 2.12. For $z \in \mathbb{C}$, let

$$w = w(z) := \text{dist}(z, (-\infty, 0]).$$

For $C \geq 0$, let $\mathcal{D}_C(B) := \{z \in \mathbb{C} : w(z) \geq c\}$, where $c \geq 1$ is the minimal choice, such that

$$C w^{-\frac{1}{2}} + (\rho_1^{-2N}(B) + \rho_1^{2N}(B) + 1)(\rho_z^{-2N}(B) + \rho_z^{2N}(B)) \leq \frac{1}{2}, \quad z \in \mathcal{D}_C(B).$$

Definition 2.15. For $s \in \mathbb{R}$, denote by Sym_s those smooth functions $f : \mathbb{R}^d \rightarrow \mathbb{C}$, such that, for all $\gamma \in \mathbb{N}_0^d$,

$$\langle X \rangle^{|\gamma|-s} \partial^\gamma f \in L^\infty(\mathbb{R}^d).$$

Remark 2.16. Straightforward calculation verifies

$$C_c^\infty(\mathbb{R}^d) \subset Sym_{-\infty} := \bigcap_{j=0}^{\infty} Sym_{-j},$$

and $\langle X \rangle^u \in Sym_u$ for $u \in \mathbb{R}$. For $f \in Sym_r$, $g \in Sym_s$, we also have $fg \in Sym_{r+s}$, which follows from the Leibniz rule. Moreover, for $f \in Sym_0$, the Leibniz rule, taking adjoints and complex interpolation imply that $\langle \not{D} \rangle^s f \langle \not{D} \rangle^{-s}$ have bounded extensions in $L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)$ for all $s \in \mathbb{R}$.

We discuss our first type of bounded operators involved in the factorization of Proposition 2.28.

Lemma 2.17. *There exists a universal constant C such that if B satisfies Hypothesis 2.12, and we let $t \in [0, 2]$, $s \in [-1, 1]$, $k \in \mathbb{N}$, $k \leq N$, and $r \in [-2N, 2N]$ with $r - 2(k - 1) \in [-2N, 2N]$, then the operators*

$$R := \langle M_0 \rangle^r \langle X \rangle^{-s} R_z(T)^k \langle X \rangle^s \langle M_0 \rangle^{2k-r-t} \langle \not{D} \rangle^t, \quad T \in \{H_B, DD^*, D^*D\},$$

possess extensions in $B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ with operator norm bounded by 2^k for $z \in \mathcal{D}_C(B)$.

Proof. We write $R = (\prod_{i=1}^{k-1} R_i)S$, with

$$S = \langle M_0 \rangle^{-2(k-1)+r} \langle X \rangle^{-s} R_z(T) \langle X \rangle^s \langle M_0 \rangle^{2k-r-t} \langle \not{D} \rangle^t,$$

$$R_i = \langle M_0 \rangle^{-2(i-1)+r} \langle X \rangle^{-s} R_z(T) \langle X \rangle^s \langle M_0 \rangle^{2i-r}, \quad i \in \{1, \dots, k-1\}.$$

We develop $R_z(T)$ into a Neumann series around H_0 ,

$$R_i = \sum_{l=0}^{\infty} (-1)^l (R_z(H_0) C_i)^l \langle M_0 \rangle^2 R_z(H_0),$$

$$S = \sum_{l=0}^{\infty} (-1)^l (R_z(H_0) C_k)^l \langle M_0 \rangle^{2-t} \langle \not{D} \rangle^t R_z(H_0),$$
(17)

where

$$C_i := \langle M_0 \rangle^{-2(i-1)+r} (B^2 + BM_0 + M_0B + \varepsilon i \not{D}^E B + \langle X \rangle^{-s} [\Delta, \langle X \rangle^s]) \langle M_0 \rangle^{2(i-1)-r},$$

where $\varepsilon = -1$ for $T = D^*D$, $\varepsilon = 0$ for $T = H_B$, and $\varepsilon = 1$ for $T = DD^*$. Since $\langle X \rangle^s \in \text{Sym}_s$, it follows that $\langle X \rangle^{-s} [\Delta, \langle X \rangle^s]$ is a first-order differential operator with coefficients in Sym_{-1} . Thus, there exists a universal constant C such that, for $u \in [-1, 1]$, $z \in \mathbb{C} \setminus (-\infty, 0]$ with $w := \text{dist}(z, (-\infty, 0]) \geq 1$,

$$\| \overline{R_z(H_0) \langle X \rangle^{-s} [\Delta, \langle X \rangle^s]} \|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))} \leq C w^{-\frac{1}{2}}.$$

Furthermore, we have by Hypothesis 2.12 the norm estimate

$$\begin{aligned} \| \overline{R_z(H_0) C_i} \|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))} &\leq C w^{-\frac{1}{2}} + \| \langle M_0 \rangle \langle M_0 \rangle_z R_z(H_0) \|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))} \\ &\cdot \| \langle M_0 \rangle_z^{-1} \langle M_0 \rangle^{-2(i-1)+r-1} (B^2 + BM_0 + M_0B + \varepsilon i \not{D} B) \langle M_0 \rangle^{2(i-1)-r} \|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))} \\ &\leq C w^{-\frac{1}{2}} + (\rho_1^{2(i-1)-r} (B) + 1) \rho_z^{2(i-1)-r} (B) \leq \frac{1}{2}, \quad z \in \mathcal{D}_C(B), \end{aligned}$$

where the last inequality follows by Remark 2.5 and the definition of the domain $\mathcal{D}_C(B)$. This implies that the Neumann series of R_i and S converge in operator norm, each of which can be bounded in operator norm by 2 for $z \in \mathcal{D}_C(B)$. We conclude that $\|\bar{R}\|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))} \leq 2^k$ for $z \in \mathcal{D}_C(B)$. ■

A similar result holds under weaker conditions, which we will need later in the proof of the approximation statement.

Lemma 2.18. *Let $B : \mathbb{R}^d \rightarrow B(H)$ be a point-wise self-adjoint C^1 -function with respect to the strong operator topology such that*

$$\|B\|_{C_b^1(\mathbb{R}^d, B(H))} = \|B\|_{L^\infty(\mathbb{R}^d, B(H))} + \|\nabla B\|_{L^\infty(\mathbb{R}^d, B(H)^d)} < \infty.$$

Assume also that $B \in C_b^1(\mathbb{R}^d, A_0, 1)$ with $\lim_{w \rightarrow \infty} \rho_z(B) = 0$, where

$$w := \text{dist}(z, (-\infty, 0]).$$

Let $t \in [0, 2]$, $s \in [-1, 1]$, and $k \in \mathbb{N}$. Then, the operators

$$R_{k,s,t} := \langle X \rangle^{-s} R_z(H_B)^k \langle X \rangle^s \langle \not{t} \rangle^t$$

admit extensions in $B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ with norm bounded by

$$C^k (\|B\|_{C_b^1(\mathbb{R}^d, B(H))} + 1)^{2k}$$

for $w \geq C(\|B\|_{C_b^1(\mathbb{R}^d, B(H))} + 1)^4$, where C is some universal constant.

For $T_B \in \{H_B, D_B^* D_B, D_B D_B^*\}$, and $w \geq C(\|B\|_{C_b^1(\mathbb{R}^d, B(H))} + 1)^4$, the operators

$$(H_0 + 1)^{\frac{1}{2}} \langle X \rangle^{-s} R_z(T_B) \langle X \rangle^s (H_0 + 1)^{\frac{1}{2}}, \quad s \in [-1, 1],$$

admit extensions in $B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ with norm bounded by

$$C^k (\|B\|_{C_b^1(\mathbb{R}^d, B(H))} + 1)^{2k}$$

for $w \geq C(\|B\|_{C_b^1(\mathbb{R}^d, B(H))} + 1)^4$.

Proof. We note that by Proposition 2.6 the operators $T_B \geq 0$ are self-adjoint, so that the involved resolvents are well defined. We show first that

$$(H_0 + 1)^{\frac{1}{2}} \langle X \rangle^{-s} R_z(T_B) \langle X \rangle^s (H_0 + 1)^{\frac{1}{2}}$$

admits a bounded extension. We develop $\langle X \rangle^{-s} R_z(T_B) \langle X \rangle^s$ into a Neumann series around H_0 :

$$\begin{aligned} & \overline{(H_0 + 1)^{\frac{1}{2}} \langle X \rangle^{-s} R_z(T_B) \langle X \rangle^s (H_0 + 1)^{\frac{1}{2}}} \\ &= (H_0 + 1)^{\frac{1}{2}} R_z(H_0)^{\frac{1}{2}} \sum_{l=0}^{\infty} (-1)^l (R_z(H_0)^{\frac{1}{2}} T_\varepsilon R_z(H_0)^{\frac{1}{2}})^l (H_0 + 1)^{\frac{1}{2}} R_z(H_0)^{\frac{1}{2}}, \end{aligned} \quad (18)$$

where

$$\begin{aligned} T_\varepsilon &:= B^2 + B M_0 + M_0 B + f_s \not{t} + g_s + i\varepsilon(\not{t} B), \\ f_s &:= 2\langle X \rangle^{-s} \not{t} \langle X \rangle^s, \\ g_s &:= \langle X \rangle^{-s} \Delta \langle X \rangle^s, \end{aligned}$$

where $\varepsilon = -1$ for $T_B = D_B^* D_B$, $\varepsilon = 0$ for $T_B = H_B$, and $\varepsilon = 1$ for $T_B = D_B D_B^*$. Since $(H_0 + 1)^{\frac{1}{2}} R_z(H_0)^{\frac{1}{2}}$ is bounded in operator norm by 1 for $w \geq 1$, it remains to

investigate the inner factor of the left-hand side of (18), and thus, we consider

$$\begin{aligned}
 R_z(H_0)^{\frac{1}{2}} T_\varepsilon R_z(H_0)^{\frac{1}{2}} &= R_z(H_0)^{\frac{1}{2}} B^2 R_z(H_0)^{\frac{1}{2}} \\
 &\quad + R_z(H_0)^{\frac{1}{2}} B M_0 R_z(H_0)^{\frac{1}{2}} \\
 &\quad + M_0 R_z(H_0)^{\frac{1}{2}} B R_z(H_0)^{\frac{1}{2}} \\
 &\quad + R_z(H_0)^{\frac{1}{2}} f_s \not B R_z(H_0)^{\frac{1}{2}} \\
 &\quad + R_z(H_0)^{\frac{1}{2}} g_s R_z(H_0)^{\frac{1}{2}} \\
 &\quad + i\varepsilon R_z(H_0)^{\frac{1}{2}} (\not B) R_z(H_0)^{\frac{1}{2}}.
 \end{aligned}$$

Since $M_0 R_z(H_0)^{\frac{1}{2}}$ and $\not B R_z(H_0)^{\frac{1}{2}}$ are uniformly bounded in operator norm by 1 for $w \geq 1$, B , B^2 , $(\not B)$ are bounded in norm operator norm by $(\|B\|_{C_b^1(\mathbb{R}^d, B(H))} + 1)^2$, and the functions $f_s \in Sym_{-1}$, $g_s \in Sym_{-2}$ give rise to uniformly bounded operators in operator norm for $s \in [-1, 1]$, the operator $R_z(H_0)^{\frac{1}{2}} T R_z(H_0)^{\frac{1}{2}}$ is uniformly bounded in operator norm by $c(\|B\|_{C_b^1(\mathbb{R}^d, B(H))} + 1)^2 w^{-\frac{1}{2}}$ for some universal constant c and $w \geq 1$. We assume for the rest of the proof that $w \geq c^2(\|B\|_{C_b^1(\mathbb{R}^d, B(H))} + 1)^4$. Then, the Neumann series (18) converges in operator norm to a bounded operator with norm bound 2. Since $(i + \not B)(H_0 + 1)^{-\frac{1}{2}}$ is bounded in operator norm by 1, we also have that

$$\overline{(i + \not B)\langle X \rangle^{-s} R_z(H_B)\langle X \rangle^s (i + \not B)} \quad (19)$$

is a bounded operator with norm less than 2. In (19), we commute $i + \not B$ and obtain

$$\begin{aligned}
 &\overline{(i + \not B)\langle X \rangle^{-s} R_z(H_B)\langle X \rangle^s (i + \not B)} \\
 &= \overline{\langle X \rangle^{-s} R_z(H_B)\langle X \rangle^s (i + \not B)^2} + \overline{[\not B, \langle X \rangle^{-s} R_z(H_B)\langle X \rangle^s] (i + \not B)}. \quad (20)
 \end{aligned}$$

By the resolvent identity, we rewrite the commutator and obtain

$$\begin{aligned}
 &\overline{[\not B, \langle X \rangle^{-s} R_z(H_B)\langle X \rangle^s] (i + \not B)} \\
 &= -\overline{\langle X \rangle^{-s} R_z(H_B)\langle X \rangle^s [\not B, T] \langle X \rangle^{-s} R_z(H_B)\langle X \rangle^s (i + \not B)} \\
 &= -\overline{\langle X \rangle^{-s} R_z(H_B)\langle X \rangle^s (H_0 + 1)^{\frac{1}{2}}} \\
 &\quad \overline{(H_0 + 1)^{-\frac{1}{2}} ((\not B B^2) + M_0(\not B) + (\not B)M_0 + (\not B f_s)\not B + (\not B g_s))(H_0 + 1)^{-\frac{1}{2}}} \\
 &\quad \overline{(H_0 + 1)^{\frac{1}{2}} \langle X \rangle^{-s} R_z(H_B)\langle X \rangle^s (i + \not B)}. \quad (21)
 \end{aligned}$$

The first and third factors of (21) are both bounded in operator norm by 2 according to the previous considerations, the second factor is bounded since $M_0 R_z(H_0)^{\frac{1}{2}}$ and $\not B R_z(H_0)^{\frac{1}{2}}$ are uniformly bounded in operator norm by 1 for $w \geq 1$, $(\not B)$, and $(\not B B^2)$

are bounded by $(\|B\|_{C_b^1(\mathbb{R}^d, B(H))} + 1)^2$, and the functions $(\not\partial f_s) \in \text{Sym}_{-2}$, $(\not\partial g_s) \in \text{Sym}_{-3}$ give rise to uniformly bounded operators in operator norm for $s \in [-1, 1]$. In total, (21) implies that $\overline{[\not\partial, \langle X \rangle^{-s} R_z(H_B) \langle X \rangle^s](i + \not\partial)}$ is uniformly bounded in operator norm by $C'(\|B\|_{C_b^1(\mathbb{R}^d, B(H))} + 1)^2$ for some universal constant C' . By (20), it follows that

$$\overline{\langle X \rangle^{-s} R_z(H_B) \langle X \rangle^s (i + \not\partial)^2},$$

and thus, $\overline{R_{1,s,t}}$ is uniformly bounded by $C''(\|B\|_{C_b^1(\mathbb{R}^d, B(H))} + 1)^2$ for some universal constant C'' , and all $t \in [0, 2]$. Finally, we use the fact that

$$R_{k,s,t} = R_{1,s,0}^{k-1} R_{1,s,t}$$

to conclude the statement. ■

We will also need the following convergence statement, which is a fundamental property of Schatten–von Neumann operators.

Lemma 2.19 ([24, Lemma 3.4]). *Let $R_n, S_n, T_n, n \in \mathbb{N}$, be bounded operators in a separable Hilbert space X . For $1 \leq p < \infty$, let $S_n \in S^p(X)$, such that $\lim_{n \rightarrow \infty} S_n = S$ in $S^p(X)$ -norm. Furthermore, assume that $\lim_{n \rightarrow \infty} R_n = R$, and $\lim_{n \rightarrow \infty} T_n^* = T^*$ strongly. Then,*

$$\lim_{n \rightarrow \infty} R_n S_n T_n = RST,$$

in $S^p(X)$ -norm.

Inspired by this lemma and for our convenience, we introduce the following notation.

Definition 2.20. If T is a bounded operator, and $(T_n)_{n \in \mathbb{N}}$ is a sequence of bounded operators in a Hilbert space X , we say T_n converges in SOTA of X to T , if T_n and T_n^* converge in the strong operator topology to T , respectively, to T^* as $n \rightarrow \infty$.

Lemma 2.21. *There exists a universal constant C such that the following statement holds true. Let B satisfy Hypothesis 2.12, and let $(B_n)_{n \in \mathbb{N}}$ be a sequence of operators, each of which satisfy Hypothesis 2.12, such that $(B_n)_{n \in \mathbb{N}}$ converges in the following sense: for $\beta \in [-2N + 1, 2N - 1]$, and a.e. $x \in \mathbb{R}^d$, we have strong operator convergence in H of*

$$\langle A_0 \rangle^\beta (B_n(x) + A_0)^2 \langle A_0 \rangle^{-2-\beta} \xrightarrow{n \rightarrow \infty} \langle A_0 \rangle^\beta (B(x) + A_0)^2 \langle A_0 \rangle^{-2-\beta}, \quad (22)$$

and with $w := \text{dist}(z, (-\infty, 0])$, assume that

$$\sup_{n \in \mathbb{N}} (\rho_z^{-2N}(B_n) + \rho_z^{2N}(B_n)) \xrightarrow{w \rightarrow \infty} 0; \quad (23)$$

then, we have SOTA convergence in $L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)$ of

$$\frac{\langle M_0 \rangle^r \langle X \rangle^{-s} R_z(H_{B_n})^k \langle X \rangle^s \langle M_0 \rangle^{2k-r-t} \langle \not{p} \rangle^t}{\xrightarrow{n \rightarrow \infty} \langle M_0 \rangle^r \langle X \rangle^{-s} R_z(H_B)^k \langle X \rangle^s \langle M_0 \rangle^{2k-r-t} \langle \not{p} \rangle^t}$$

for $t \in [0, 2]$, $u \in [-1, 1]$, $k \in \mathbb{N}$, $k \leq N$, and $r \in [-2N, 2N]$ with $r - 2(k - 1) \in [-2N, 2N]$.

If additionally for a.e. $x \in \mathbb{R}^d$ we have strong operator convergence in H of

$$\langle A_0 \rangle^\beta \partial_i B_n(x) \langle A_0 \rangle^{-2-\beta} \xrightarrow{n \rightarrow \infty} \langle A_0 \rangle^\beta \partial_i B(x) \langle A_0 \rangle^{-2-\beta}, \quad i \in \{1, \dots, d\},$$

then we also have SOTA convergence in $L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)$ of

$$\frac{\langle M_0 \rangle^r \langle X \rangle^{-s} R_z(D_{B_n} D_{B_n}^*)^k \langle X \rangle^s \langle M_0 \rangle^{2k-r-t} \langle \not{p} \rangle^t}{\xrightarrow{n \rightarrow \infty} \langle M_0 \rangle^r \langle X \rangle^{-s} R_z(D_B D_B^*)^k \langle X \rangle^s \langle M_0 \rangle^{2k-r-t} \langle \not{p} \rangle^t},$$

and

$$\frac{\langle M_0 \rangle^r \langle X \rangle^{-s} R_z(D_{B_n}^* D_{B_n})^k \langle X \rangle^s \langle M_0 \rangle^{2k-r-t} \langle \not{p} \rangle^t}{\xrightarrow{n \rightarrow \infty} \langle M_0 \rangle^r \langle X \rangle^{-s} R_z(D_B^* D_B)^k \langle X \rangle^s \langle M_0 \rangle^{2k-r-t} \langle \not{p} \rangle^t},$$

for $t \in [0, 2]$, $u \in [-1, 1]$, $k \in \mathbb{N}$, $k \leq N$, and $r \in [-2N, 2N]$ with $r - 2(k - 1) \in [-2N, 2N]$.

Proof. We only show the statement involving H_B . The proof for $D_B D_B^*$ and $D_B^* D_B$ is analogous. Consider the factorization presented in the proof of Lemma 2.17, now with B_n replacing B everywhere. We note that both Neumann series in (17) converge for $z \in \mathcal{D}_C(B_n)$. Due to condition (23), there exists $w_0 \geq 1$, such that $\{z \in \mathbb{C} : w(z) \geq w_0\} \subseteq \mathcal{D}_C(B) \cap \bigcap_{n \in \mathbb{N}} \mathcal{D}_C(B_n)$. Thus, analogous to the proof of Lemma 2.17, the operators

$$S_n(t) := \langle M_0 \rangle^{-2(k-1)+r} \langle X \rangle^{-s} R_z(H_{B_n}) \langle X \rangle^s \langle M_0 \rangle^{2k-r-t} \langle \not{p} \rangle^t, \\ S(t) := \langle M_0 \rangle^{-2(k-1)+r} \langle X \rangle^{-s} R_z(H_B) \langle X \rangle^s \langle M_0 \rangle^{2k-r-t} \langle \not{p} \rangle^t$$

have bounded extensions for $w(z) \geq w_0$, where w_0 is independent of n , and their operator norms are uniformly bounded by 2. By the resolvent identity, we find

$$\overline{S_n(t)} - \overline{S(t)} \\ = \overline{S_n(0)} \overline{(\langle M_0 \rangle^{-2k+r} ((B + M_0)^2 - (B_n + M_0)^2) \langle M_0 \rangle^{2(k-1)-r}) S(t)}. \quad (24)$$

Since $\overline{S_n(0)}$ is uniformly bounded by 2, it suffices to verify the strong operator convergence in $L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)$ of the inner factor of (24) to conclude the strong operator

convergence of $\overline{S_n(t)}$ to $\overline{S(t)}$. Indeed, condition (22), the uniform bound given by condition (23), and the dominated convergence theorem ensure the strong convergence of the inner factor. For the remaining factors

$$R_{i,n} := \langle M_0 \rangle^{-2(i-1)+r} \langle X \rangle^{-s} R_z(H_{B_n}) \langle X \rangle^s \langle M_0 \rangle^{2i-r},$$

we obtain analogous results. For the strong convergence of the adjoints, the claimed statement follows similarly if one replaces (24) with

$$\begin{aligned} S_n(t)^* - S(t)^* \\ = S_n(t)^* \overline{\langle M_0 \rangle^{2(k-1)-r} ((B + M_0)^2 - (B_n + M_0)^2) \langle M_0 \rangle^{-2k+r} S(0)^*}, \end{aligned}$$

using the fact that the operator functions B_n and B are point-wise symmetric. ■

We also provide here a variant under weaker conditions, which we will later also need.

Lemma 2.22. *Let $B : \mathbb{R}^d \rightarrow B(H)$, $B_n : \mathbb{R}^d \rightarrow B(H)$ be point-wise self-adjoint C^1 -functions with respect to the strong operator topology for $n \in \mathbb{N}$, and assume that $\|B\|_{C_b^1(\mathbb{R}^d, B(H))}$ and $\|B_n\|_{C_b^1(\mathbb{R}^d, B(H))}$ are uniformly bounded. Assume also that $B, B_n \in C_b^1(\mathbb{R}^d, A_0, 1)$, and that, for all $n \in \mathbb{N}$,*

$$\lim_{w \rightarrow \infty} \rho_z(B) = \lim_{w \rightarrow \infty} \rho_z(B_n) = 0,$$

where

$$w := \text{dist}(z, (-\infty, 0]).$$

Finally, assume that $B_n(x) \xrightarrow{n \rightarrow \infty} B(x)$ and $\nabla B_n(x) \xrightarrow{n \rightarrow \infty} \nabla B(x)$ for a.e. $x \in \mathbb{R}^d$ in the strong operator topology in H . Then, there exist constants c and C such that for

$$w := \text{dist}(z, (-\infty, 0]) \geq c$$

we have convergence in strong operator topology of $L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)$ of

$$\overline{\langle X \rangle^{-s} R_z(H_{B_n})^k \langle X \rangle^s \langle \not{D} \rangle^t} \xrightarrow{n \rightarrow \infty} \overline{\langle X \rangle^{-s} R_z(H_B)^k \langle X \rangle^s \langle \not{D} \rangle^t} \quad (25)$$

for $t \in [0, 2]$, $s \in [-1, 1]$, and $k \in \mathbb{N}$, and the operators are uniformly bounded in operator norm by C . In case $t = 0$, (25) converges in SOTA of $L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)$. Moreover, for $w \geq 1$, we have SOTA convergence in $L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)$ of

$$\begin{aligned} R_z(D_{B_n}^* D_{B_n})^k &\xrightarrow{n \rightarrow \infty} R_z(D_B^* D_B)^k, \\ R_z(D_{B_n} D_{B_n}^*)^k &\xrightarrow{n \rightarrow \infty} R_z(D_B D_B^*)^k. \end{aligned} \quad (26)$$

Proof. By the uniform boundedness principle and Lemma 2.18, there exist constants c, C such that for $w \geq c$ we have the uniform bound

$$\begin{aligned} & \left\| \overline{\langle X \rangle^{-s} R_z (H_{B_n})^k \langle X \rangle^s \langle \not{p} \rangle^t} \right\|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))}, \\ & \left\| \overline{\langle X \rangle^{-s} R_z (H_B)^k \langle X \rangle^s \langle \not{p} \rangle^t} \right\|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))} \leq C. \end{aligned}$$

It suffices to restrict to the case $k = 1$ by factorizing the operators. Due to the uniform norm bounds and the density of $C_c^\infty(\mathbb{R}^d)$ in $L^2(\mathbb{R}^d)$, we may also assume $t = 0$. Then, with

$$S_n := \overline{\langle X \rangle^{-s} R_z (H_{B_n}) \langle X \rangle^s}, \quad S := \overline{\langle X \rangle^{-s} R_z (H_B) \langle X \rangle^s},$$

the resolvent identity implies

$$S_n - S = S_n ((B + M_0)^2 - (B_n + M_0)^2) S.$$

Since the operators $\overline{S_n M_0}$, $M_0 S$ are uniformly bounded by Lemma 2.18, it follows that S_n converges in the strong operator topology to S .

For the convergence of the adjoints of (25) in case $t = 0$, we similarly may restrict to the case $k = 1$, and by the resolvent identity, we have

$$S_n^* - S^* = S_n^* ((B + M_0)^2 - (B_n + M_0)^2) S^*. \quad (27)$$

Since $\overline{S_n^* M_0}$, $M_0 S^*$ are uniformly bounded by Lemma 2.18, (27) also converges in strong operator topology.

It remains to investigate the SOTA convergence of (26). It suffices to show convergence in strong operator convergence for $k = 1$ since we may factorize and taking adjoints only changes z to $\bar{z}$. The statement then follows as before by the resolvent identity and the uniform norm bounds provided by Lemma 2.18. ■

We now present results on the type of operators that we will encounter as Schatten-von Neumann class factors in the proof of Proposition 2.28.

Lemma 2.23. *Let B satisfy Hypothesis 2.12, let $\phi \in C_c^\infty(\mathbb{R}^d)$, $0 \leq \phi \leq 1$, $\text{supp } \phi \subseteq \overline{B_1(0)}$ and $\phi \equiv 1$ on $\overline{B_{\frac{1}{2}}(0)}$, and let $\beta \in \mathbb{R}$ satisfy $|\beta - \alpha| \leq 2N$, and $|\beta - 1| \leq 2N$. Then, there exist $\varepsilon > 0$ such that, for all $\delta > 0$,*

$$\langle \not{p} \rangle^{-1-\delta} \langle M_0 \rangle^{\beta-\alpha} \langle X \rangle^\varepsilon (\phi i(\not{p} B) + (1 - \phi) i c_R(\partial_R B)) \langle M_0 \rangle^{-\beta} \quad (28)$$

possesses an $S^d(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ -extension. On the other hand, for all $\varepsilon, \delta > 0$,

$$\langle \not{p} \rangle^{-1-\delta} \langle M_0 \rangle^{\beta-\alpha} \langle X \rangle^{-\varepsilon} (\phi i(\not{p} B) + (1 - \phi) i c_R(\partial_R B)) \langle M_0 \rangle^{-\beta} \quad (29)$$

and

$$\langle \not{J} \rangle^{-1-\delta} \langle M_0 \rangle^{\beta-\alpha} \langle X \rangle^{-\varepsilon} (1-\phi) i((\not{J} - c_R \partial_R) B) \langle M_0 \rangle^{-\beta} \quad (30)$$

possess $S^d(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ -extensions. Finally, for all $\delta > 0$,

$$\langle \not{J} \rangle^{-1} \langle M_0 \rangle^{\beta-\alpha} i(\not{J} B) \langle M_0 \rangle^{-\beta} \quad (31)$$

possesses an $S^{d+\delta}(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ -extension.

Proof. We first consider (28). We note that due to the compact support of ϕ , for $\varepsilon > 0$, there is a constant C , such that

$$\begin{aligned} & \left\| \langle M_0 \rangle^{-\alpha+\beta} \langle X \rangle^\varepsilon (\phi i(\not{J} B) + (1-\phi) i c_R(\partial_R B)) \langle M_0 \rangle^{-\beta} \right\|_{L^d(S^d(H))} \\ & \leq C(\tau^{\alpha,\beta,\nabla,d,1}(B) + \tau^{\alpha,\beta,\partial_R,d,1+2\varepsilon}(B)), \end{aligned}$$

which is finite for $\varepsilon > 0$ small enough, due to Hypothesis 2.12. For (29) and (30), we similarly have for all $\varepsilon > 0$ a constant C , such that

$$\begin{aligned} & \left\| \langle M_0 \rangle^{\beta-\alpha} \langle X \rangle^{-\varepsilon} (\phi i(\not{J} B) + (1-\phi) i c_R(\partial_R B)) \langle M_0 \rangle^{-\beta} \right\|_{L^d(S^d(H))} \\ & + \left\| \langle M_0 \rangle^{\beta-\alpha} \langle X \rangle^{-\varepsilon} (1-\phi) i((\not{J} - c_R \partial_R) B) \langle M_0 \rangle^{-\beta} \right\|_{L^d(S^d(H))} \\ & \leq C \tau^{\alpha,\beta,\nabla,d,1}(B), \end{aligned}$$

which is also finite by Hypothesis 2.12. For (31), we have, for all $\delta > 0$, a constant C , such that

$$\left\| \langle M_0 \rangle^{\beta-\alpha} i(\not{J} B) \langle M_0 \rangle^{-\beta} \right\|_{L^{d+\delta}(S^{d+\delta}(H))} \leq C \tau^{\alpha,\beta,\nabla,d,1}(B),$$

which is finite by Hypothesis 2.12. The claims now follow from Corollary 2.9 and $\langle X \rangle^{-1-\delta} \in L^d(\mathbb{R}^d)$, respectively, $\langle X \rangle^{-1} \in L^{d+\delta}(\mathbb{R}^d)$, for all $\delta > 0$. ■

In a similar manner, one shows the weaker result under weaker conditions on the operator family B below.

Lemma 2.24. *Let $B : \mathbb{R}^d \rightarrow B(H)$ be a point-wise self-adjoint C^1 -function with respect to the strong operator topology, and assume that there exists $\eta > 0$, such that*

$$\tau^{0,0,\nabla,d,1}(B) + \tau^{0,0,\partial_R,d,1+\eta}(B) < \infty.$$

Let $\phi \in C_c^\infty(\mathbb{R}^d)$, $0 \leq \phi \leq 1$, $\text{supp } \phi \subseteq \overline{B_1(0)}$, and $\phi \equiv 1$ on $\overline{B_{\frac{1}{2}}(0)}$. Then, there exist $\varepsilon > 0$ such that, for all $\delta > 0$,

$$\langle \not{J} \rangle^{-1-\delta} \langle X \rangle^\varepsilon (\phi i(\not{J} B) + (1-\phi) i c_R(\partial_R B))$$

possesses an $S^d(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ -extension. On the other hand, for all $\varepsilon, \delta > 0$,

$$\langle \not{J} \rangle^{-1-\delta} \langle X \rangle^{-\varepsilon} (\phi i(\not{J} B) + (1-\phi) i c_R(\partial_R B))$$

and

$$\langle \not{\partial} \rangle^{-1-\delta} \langle X \rangle^{-\varepsilon} (1 - \phi) i((\not{\partial} - c_R \partial_R) B)$$

possess $S^d(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ -extensions. Finally, for all $\delta > 0$,

$$\langle \not{\partial} \rangle^{-1} i(\not{\partial} B)$$

possesses a $S^{d+\delta}(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ -extension.

In the next lemma, we prepare the upcoming factorizations of Proposition 2.28. We will utilize the following notation.

Definition 2.25. Let $l \in \mathbb{N}$. For Y a Banach space, define the shuffle product $\sqcup$ between $l+1$ -tuples of operators $T = (T_0, \dots, T_l)$ in Y , and l -tuples of operators $S = (S_1, \dots, S_l)$ in Y by

$$T \sqcup S := T_0 S_1 T_1 \cdots S_l T_l.$$

For T an operator in Y , $S = (S_1, \dots, S_l)$ an l -tuple of operators in Y , and $k \in \{1, \dots, l+1\}$, denote

$$\begin{aligned} \iota_T^k S &:= (S_1, \dots, S_{k-1}, T, S_k, \dots, S_l), \quad k \leq l, \\ \iota_T^{l+1} S &:= (S_1, \dots, S_l, T). \end{aligned}$$

Denote for a sequence of operators $(S_k)_{k \in \mathbb{N}_0}$ and $\eta \in \mathbb{N}_0^l$ by S^η the l -tuple of operators

$$S^\eta := (S_{\eta_1}, \dots, S_{\eta_l}).$$

Finally, denote $\mathbb{1} := (1, \dots, 1) \in \mathbb{N}^l$.

Lemma 2.26. Assume Hypothesis 2.12. Let $z \in \mathbb{C} \setminus (-\infty, 0]$. Then,

$$\begin{aligned} & \operatorname{tr}_{\mathbb{C}^r} (R_z(D_B^* D_B)^N - R_z(D_B D_B^*)^N) \\ &= 2 \operatorname{tr}_{\mathbb{C}^r} \sum_{\substack{\gamma \in \mathbb{N}^{d+1} \\ |\gamma| = N+d}} \binom{N-1}{\gamma - \mathbb{1}}^{-1} R_z(H_B)^\gamma \sqcup (i \not{\partial} B)^{\otimes d} \\ &+ \operatorname{tr}_{\mathbb{C}^r} \sum_{\substack{\gamma \in \mathbb{N}^{d+3} \\ |\gamma| = N+d+2}} \binom{N-1}{\gamma - \mathbb{1}}^{-1} ((R_z(H_B)^{\otimes(d+2)}, R_z(D_B^* D_B))^\gamma \sqcup (i \not{\partial} B)^{\otimes(d+2)} \\ &+ (R_z(H_B)^{\otimes(d+2)}, R_z(D_B D_B^*))^\gamma \sqcup (i \not{\partial} B)^{\otimes(d+2)}). \end{aligned}$$

Proof. By Hypothesis 2.12 and Proposition 2.6, we have, for $w = \operatorname{dist}(z, (-\infty, 0])$ large enough,

$$\|i \not{\partial} B R_z(H_B)\|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))} \leq w^{-\frac{1}{2}} \rho_z^1(B) < 1.$$

We may develop the Neumann series of $R_z(D_B D_B^*)$ and $R_z(D_B^* D_B)$ and obtain

$$\begin{aligned} R_z(D_B^* D_B) - R_z(D_B D_B^*) &= 2R_z(H_B) \sum_{k=0}^{\infty} (i(\not\partial B) R_z(H_B))^{2k+1}, \\ R_z(D_B^* D_B) + R_z(D_B D_B^*) &= 2R_z(H_B) \sum_{k=0}^{\infty} (i(\not\partial B) R_z(H_B))^{2k}. \end{aligned}$$

So, by Lemma 2.1, we have, for w large enough,

$$\begin{aligned} \mathrm{tr}_{\mathbb{C}^r} (R_z(D_B^* D_B) - R_z(D_B D_B^*)) \\ = 2\mathrm{tr}_{\mathbb{C}^r} R_z(H_B) (i(\not\partial B) R_z(H_B))^d \sum_{k=0}^{\infty} (i(\not\partial B) R_z(H_B))^{2k} \\ = \mathrm{tr}_{\mathbb{C}^r} (R_z(H_B) i(\not\partial B))^d (R_z(D_B^* D_B) + R_z(D_B D_B^*)); \end{aligned} \quad (32)$$

both sides are holomorphic on $\mathbb{C} \setminus [0, \infty)$, which implies that the above identity extends to this domain. Differentiating (32) $(N-1)$ -times in z yields the claim. ■

We now arrive at the principal decomposition result. However, we will first introduce further abbreviations for the involved operators.

Definition 2.27. Let $k, l, m \in \mathbb{N}_0$, $\beta \in \mathbb{R}^{l+1}$, $\gamma \in \mathbb{N}^{l+1}$, $\varepsilon \in \mathbb{R}^l$, $\zeta \in \{0, 1, 2\}^l$, $\alpha \geq 0$, and $\delta, \xi > 0$. For an operator family B satisfying Hypothesis 2.12, define the operators

$$\begin{aligned} T(B)^0 &:= \phi i(\not\partial B) + (1 - \phi) i c_R(\partial_R B), \\ T(B)^1 &:= (1 - \phi) i((\not\partial - c_R \partial_R) B), \\ T(B)^2 &:= i(\not\partial B) = T(B)^0 + T(B)^1, \\ L &:= [\Delta, (1 - \psi) c_R]. \end{aligned}$$

Now, define the operators for $m \in \{1, \dots, \gamma_k\}$,

$$\begin{aligned} u_z^{a,b,c,d,k}(B) &:= \langle M_0 \rangle^a \langle X \rangle^b R_z(H_B)^k \langle X \rangle^{-b} \langle M_0 \rangle^c \langle \not\partial \rangle^d, \\ a, b, c, d &\in \mathbb{R}, \quad k \in \mathbb{N}, \\ (U_z(B)^{\alpha,\beta,\gamma,\delta,\varepsilon})_i &:= u_z^{\beta_i, \varepsilon_i, 2\gamma_i - 1 - \delta - \beta_i, 1 + \delta, \gamma_i}(B), \quad 0 \leq i \leq l-1, \\ (U_z(B)^{\alpha,\beta,\gamma,\delta,\varepsilon})_l &:= u_z^{\beta_l, 0, 0, 0, \gamma_l}(B), \\ (V(B)^{\alpha,\beta,\delta,\varepsilon,\xi})_i &:= \langle \not\partial \rangle^{-1-\delta} \langle M_0 \rangle^{\beta_i - \alpha} \langle X \rangle^{\varepsilon_i} T(B)^{\xi_i} \langle M_0 \rangle^{-\beta_i}, \quad i \in \{1, \dots, l\}, \\ (W_z(B)^{\alpha,\beta,\gamma,\delta,\xi,k,m})_i &:= u_z^{\beta_i, -i\xi, 2\gamma_i - 1 - \delta - \beta_i, 1 + \delta, \gamma_i}(B), \quad 0 \leq i < k \leq d, \\ (W_z(B)^{\alpha,\beta,\gamma,\delta,\xi,k,m})_i &:= u_z^{\beta_i, -(d-i)\xi, 2\gamma_i - 1 - \delta - \beta_i, 1 + \delta, \gamma_i}(B), \quad k < i < d, \\ (W_z(B)^{\alpha,\beta,\gamma,\delta,\xi,k,m})_d &:= u_z^{\beta_d, 0, 0, 0, \gamma_d}(B), \quad k < d, \end{aligned}$$

$$\begin{aligned}
(W_z(B)^{\alpha,\beta,\gamma,\delta,\xi,k,m})_k &:= u_z^{\beta_k,k\xi,2m-1-\beta_k,1,m}(B)(\langle\beta\rangle^{-1}\langle X\rangle^{k\xi}L\langle X\rangle^{(d-k)\xi}) \\
&\quad u_z^{\beta_k+1-2m,-(d-k)\xi,2\gamma_k-1-\beta_k-\delta,1+\delta,\gamma_k-m+1}(B), \\
0 &\leq k \leq d-1, \\
(W_z(B)^{\alpha,\gamma,\delta,\xi,d,m})_d &:= u_z^{\beta_d,d\xi,2m-1-\beta_d,1,m}(B)(\langle\beta\rangle^{-1}\langle X\rangle^{d\xi}L) \\
&\quad \times u_z^{\beta_d+1-2m,0,0,0,\gamma_d-m+1}(B).
\end{aligned}$$

The next proposition is the central result of this section. It is similar to the central result obtained in [22], where the statement below was shown without the presence of the partial trace $\mathrm{tr}_{\mathbb{C}^r}$, but with much stronger assumptions on the family A , which are not sensible for the calculation of the principal trace. In fact, if we would take the intersection of Hypothesis 2.12 and the assumptions made in [22], we would always end up with the trivial case

$$\mathrm{tr}_{L^2(\mathbb{R}^d,H)}\mathrm{tr}_{\mathbb{C}^r}(e^{-tD^*D} - e^{-tDD^*}) = 0.$$

Proposition 2.28. *There exists a universal constant C such that the following holds true. Assume Hypothesis 2.12. Let $\psi, \phi \in C_c^\infty(\mathbb{R}^d)$, with $0 \leq \psi, \phi \leq 1$, $\mathrm{supp} \psi \subseteq \overline{B_{\frac{1}{2}}(0)}$, and $\psi \equiv 1$ on $\overline{B_{\frac{1}{4}}(0)}$, and $\mathrm{supp} \phi \subseteq \overline{B_1(0)}$, and $\phi \equiv 1$ on $\overline{B_{\frac{1}{2}}(0)}$. Then, there exist, independent of the choices of B, ψ, ϕ , and $z \in \mathcal{D}_C(B)$, multi-indices $\beta \in [\alpha - 2N, \alpha + 2N] \cap [1 - 2N, -1 + 2N]$, $\varepsilon^j, \eta^j \in [-1, 1]^d$ for $j \in \{1, \dots, 5\}$, constants $\delta, \xi \in [0, 1]$, and $C_\gamma^j, C_{\gamma,k} < \infty$ for $\gamma \in \mathbb{N}^{d+1}$, $k \in \{0, \dots, d\}$, $j \in \{1, 2, 3\}$, such that*

$$\begin{aligned}
&\mathrm{tr}_{\mathbb{C}^r}(R_z(D_B^*D_B)^N - R_z(D_B D_B^*)^N) \\
&= \mathrm{tr}_{\mathbb{C}^r} \left[\sum_{\substack{\gamma \in \mathbb{N}^{d+1} \\ |\gamma|=N+d}} C_\gamma^1 \sum_{\substack{\xi \in \{0,1\}^d \\ |\xi| \leq d-1}} U_z^{\alpha,\beta,\gamma,\delta,\varepsilon^1}(B) \sqcup V^{\alpha,\beta,\delta,\eta^1,\xi}(B) \right] \\
&\quad + \mathrm{tr}_{\mathbb{C}^r} \left[\sum_{\substack{\gamma \in \mathbb{N}^{d+1} \\ |\gamma|=N+d}} C_\gamma^2 ((1-\phi)U_z(B)^{\alpha,\beta,\gamma,\delta,\varepsilon^2} \sqcup V(B)^{\alpha,\beta,\delta,\eta^2,\mathbb{1}} \phi \right. \\
&\quad \left. + \phi U_z(B)^{\alpha,\beta,\gamma,\delta,\varepsilon^3} \sqcup V(B)^{\alpha,\beta,\delta,\eta^3,\mathbb{1}}) \right] \\
&\quad + \mathrm{tr}_{\mathbb{C}^r} \left[c_R(1-\phi) \sum_{\substack{\gamma \in \mathbb{N}^{d+1} \\ |\gamma|=N+d}} \sum_{k=0}^d C_{\gamma,k} \sum_{m=1}^{\gamma_k} W_z(B)^{\alpha,\beta,\gamma,\delta,\xi,k,m} \sqcup V(B)^{\alpha,\beta,\delta,\eta^4,\mathbb{1}} \right] \\
&\quad + \mathrm{tr}_{\mathbb{C}^r} \left[\sum_{\substack{\gamma=(\hat{\gamma},\gamma_d+2) \in \mathbb{N}^{d+2} \times \mathbb{N} \\ |\gamma|=N+d+2}} C_\gamma^3 (U_z^{\alpha,\beta,\hat{\gamma},0,0}(B) \sqcup V^{\alpha,\beta,0,0,2,\mathbb{1}}) \right. \\
&\quad \left. \cdot i(\beta B)(R_z(D_B^*D_B)^{\gamma_d+2} + R_z(D_B D_B^*)^{\gamma_d+2}) \right], \quad z \in \mathcal{D}_C(B),
\end{aligned}$$

where each summand in $[\cdot]$ -brackets is a trace-class operator in $L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)$ with trace norm bound given by a z -independent polynomial in

$$\tau^{\alpha, \beta, \nabla, d, 1}(B) + \tau^{\alpha, \beta, \partial_R, d, 1+\chi}(B), \quad (33)$$

for β running over z -independent finite subsets of $[\alpha - 2N, \alpha + 2N] \cap [1 - 2N, -1 + 2N]$, and some z -independent $\chi > 0$ small enough, such that (33) is finite.

Proof. We continue with the formula from Lemma 2.26 and further decompose the involved terms. First, we start with the sum indexed by $\gamma \in \mathbb{N}^{d+1}$, $|\gamma| = N + d$, whose summands, up to factors only dependent on γ and N , are

$$R_z(H_B)^\gamma \sqcup (\mathfrak{i}\not B)^{\otimes d}. \quad (34)$$

If we expand $\mathfrak{i}(\not B) = T(B)^2 = T(B)^0 + T(B)^1$ in (34), we obtain $2^d - 1$ summands, where at least one $T(B)^0$ appears, and one summand which only involves $T(B)^1$. The summands which do involve $T(B)^0$ can be decomposed as

$$U_z^{\alpha, \beta, \gamma, \delta, \varepsilon^1}(B) \sqcup V^{\alpha, \beta, \delta, \varepsilon^1, \zeta}(B),$$

where $\zeta \in \{0, 1\}^d$, $|\zeta| \leq d - 1$, and β , δ , ε^1 , and η^1 are chosen as follows. Let $j \in \{0, \dots, d\}$ such that $\zeta_j = 0$. For $\delta > 0$, set $\beta_0 := 0$, $\beta_{i+1} := \beta_i + \alpha + \delta + 1 - 2\gamma_i$. For $\xi > 0$, set $\varepsilon_i^1 := i\xi$ for $0 \leq i \leq j - 1$, and $\varepsilon_i^1 := -(d - i)\xi$ for $j \leq i \leq d - 1$. Set $\eta_i^1 := -\xi$ for $i \neq j$, and $\eta_j^1 := d\xi$. Choose $\xi > 0$ small enough such that $(V^{\alpha, \beta, \delta, \eta^1, \zeta}(B))_i \in S^d(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ for all i , which exists according to Lemma 2.23. Lemma 2.17, on the other hand, ensures that $(U_z^{\alpha, \beta, \gamma, \delta, \varepsilon^1})_i \in B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$, for $0 \leq i \leq d - 1$, with operator norms bounded by 4^{γ_i} for w satisfying (33). Since $(\alpha + 1)d < 2(N + d)$ by Hypothesis 2.12, we may choose $\delta > 0$ small enough such that $\beta_d < 2\gamma_d$, which then also implies that $(U_z^{\alpha, \beta, \gamma, \delta, \varepsilon^1})_d \in B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ by Lemma 2.17.

Next, we decompose

$$T := R_z(H_B)^\gamma \sqcup (T(B)^1)^{\otimes d},$$

via $T = (1 - \phi)T\phi + \phi T + (1 - \phi)T(1 - \phi)$. Those summands which do involve a factor ϕ can be written as

$$(1 - \phi)[U_z(B)^{\alpha, \beta, \gamma, \delta, \varepsilon^2} \sqcup V(B)^{\alpha, \beta, \delta, \eta^2, 1}] \phi$$

and

$$\phi[U_z(B)^{\alpha, \beta, \gamma, \delta, \varepsilon^3} \sqcup V(B)^{\alpha, \beta, \delta, \eta^3, 1}],$$

where we set $\varepsilon_i^2 := -i\xi$, and $\varepsilon_d^2 := d\xi$, $\varepsilon_i^3 := -(d - i)\xi$, and $\varepsilon_0^3 := d\xi$, and $\eta_i^2 := \eta_i^3 := -\xi$. If we choose $\delta, \xi > 0$ sufficiently small, the same reason as above implies

that we have $\overline{(U_z^{\alpha,\beta,\gamma,\delta,\varepsilon^2})_i} \in B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ for $0 \leq i \leq d-1$, $\overline{(U_z^{\alpha,\beta,\gamma,\delta,\varepsilon^2})_d} \phi \in B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$, $\phi(U_z^{\alpha,\beta,\gamma,\delta,\varepsilon^3})_0 \in B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$, and $\overline{(U_z^{\alpha,\beta,\gamma,\delta,\varepsilon^3})_i} \in B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ for $1 \leq i \leq d$, where the operator norm is bounded by 4^{γ_i} . We also have $\overline{(V^{\alpha,\beta,\delta,\eta^2,\mathbb{1}})_i}, \overline{(V^{\alpha,\beta,\delta,\eta^3,\mathbb{1}})_i} \in S^d(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$.

The remaining summand $(1 - \phi)T(1 - \phi)$ requires more work. First, note that

$$[H_B, (1 - \psi)c_R] = [\Delta, (1 - \psi)c_R] = L,$$

and thus,

$$[(1 - \psi)c_R, R_z(H_B)^n] = \sum_{m=1}^n R_z(H_B)^m L R_z(H_B)^{n-m+1}.$$

On the other hand, $(1 - \psi)c_R$ anti-commutes with $T(B)^1$, since c_R anti-commutes with $\not\partial - c_R \partial_R$, because ∂_R is a component in an orthonormal system given by coordinates. Consequently, since there is an odd number of factors $T(B)^1$, we obtain, with $\{\cdot, \cdot\}$ denoting the anti-commutator,

$$\begin{aligned} & \{(1 - \psi)c_R, T\} \\ &= \sum_{k=0}^d (-1)^k \sum_{m=1}^{\gamma_k} R_z(H_B)^{(\gamma_0, \dots, \gamma_{k-1}, m, \gamma_k - m + 1, \gamma_{k+1}, \dots, \gamma_d)} \sqcup (t_L^{k+1}(T(B)^1)^{\otimes d}). \end{aligned}$$

Applying $\text{tr}_{\mathbb{C}^r}$, and bringing c_R around, we, thus, obtain

$$\begin{aligned} & \text{tr}_{\mathbb{C}^r} (1 - \phi) R_z(H_B)^\gamma \sqcup (T(B)^1)^{\otimes d} (1 - \phi) \\ &= -\frac{1 - \phi}{2} \text{tr}_{\mathbb{C}^r} c_R \sum_{k=0}^d (-1)^k \sum_{m=1}^{\gamma_k} R_z(H_B)^{(\gamma_0, \dots, \gamma_{k-1}, m, \gamma_k - m + 1, \gamma_{k+1}, \dots, \gamma_d)} \\ & \quad \sqcup (t_L^{k+1}(T(B)^1)^{\otimes d}) \\ &= \text{tr}_{\mathbb{C}^r} c_R (1 - \phi) \sum_{k=0}^d c_{\gamma,k} \sum_{m=1}^{\gamma_k} W_z(B)^{\alpha,\beta,\gamma,\delta,\xi,k,m} \sqcup V(B)^{\alpha,\beta,\delta,\eta_4,\mathbb{1}}, \end{aligned}$$

where we set $\eta_i^4 := -\xi$. As before, $\overline{(V^{\alpha,\beta,\delta,\eta^4,\mathbb{1}})_i} \in S^d(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$, and

$$\overline{(W_z^{\alpha,\beta,\gamma,\delta,\xi,k,m})_i} \in B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$$

for $i \neq k$, with operator norm bounded by 4^{γ_i} . For $i = k$, the operator $(W_z^\bullet(B))_k$ contains two factors of the type $u_z^\bullet(B)$, which both have bounded extensions with operator norm bounded by 4^m , and $4^{\gamma_k - m}$, respectively, by Lemma 2.17. The remaining factor of $(W_z^\bullet(B))_k$ is

$$\langle \not\partial \rangle^{-1} \langle X \rangle^{k\xi} [\Delta, (1 - \psi)c_R] \langle X \rangle^{(d-k)\xi}. \quad (35)$$

Since $(1 - \psi)c_R \in \text{Sym}_0$, it follows that $\langle X \rangle^{k\xi} [\Delta, (1 - \psi)c_R] \langle X \rangle^{(d-k)\xi}$ is a first-order operator with coefficients in $\text{Sym}_{-1+d\xi} \subseteq \text{Sym}_0$ for $\xi > 0$ small enough. In particular, (35) has a bounded operator extension with operator norm C . Therefore, $(W_z^{\alpha, \beta, \gamma, \delta, \xi, k, m})_k \in B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ with operator norm bounded by $4^{\gamma k} C$.

Finally, in the formula of Lemma 2.26, we consider the remaining sum indexed by $\gamma \in \mathbb{N}^{d+3}$, $|\gamma| = N + d + 2$. The summands are up to a constant of the form

$$(R_z(H_B)^{\otimes(d+2)}, R_z(T))^\gamma \lrcorner (\not B)^{\otimes(d+2)}, \quad T \in \{DD^*, D^*D\},$$

which we factorize into

$$(U_z^{\alpha, \beta, \hat{\gamma}, 0, 0}(B) \lrcorner V^{\alpha, \beta, 0, 0, 2, \mathbb{1}}) i(\not B) \langle M_0 \rangle^{-1} \langle M_0 \rangle R_z(T)^{\gamma_{d+2}},$$

where $\hat{\gamma} := (\gamma_0, \dots, \gamma_{d+1})$, $\beta_0^2 := 0$, and $\beta_{i+1}^2 := \beta_i^2 + \alpha + 1 - \gamma_i$. As noted before, we have $(U_z^{\alpha, \beta, \hat{\gamma}, 0, 0}(B))_i \in B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ with operator norm bounded by 4^{γ_i} by Lemma 2.17. Also, $i\not B \langle M_0 \rangle^{-1} \in B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ by Hypothesis 2.12, and the fact that for measurable S , $\|S\|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))} = \|S\|_{L^\infty(\mathbb{R}^d, B(\mathbb{C}^r \otimes H))}$. Also, $\langle M_0 \rangle R_z(T)^{\gamma_{d+2}}$ is bounded with operator norm bounded by $4^{\gamma_{d+2}}$ by Lemma 2.17. On the other hand, Lemma 2.23 implies that $\overline{V_i^{\alpha, \beta, 0, 0, 2, \mathbb{1}}} \in S^{d+1}(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$.

We note that by the proof of Lemma 2.23 there exist z -independent finite sets

$$I \subset [\alpha - 2N, 2N + \alpha] \cap [1 - 2N, -1 + 2N],$$

and z -independent constants C , and $\chi > 0$ small enough, such that the S^d -respectively, S^{d+1} -norms of the various operators $\overline{V^\bullet(B)}$ can be bounded uniformly by

$$C \sum_{\beta \in I, \chi \in J} (\tau^{\alpha, \beta, \nabla, d, 1}(B) + \tau^{\alpha, \beta, \partial_R, d, 1+\chi}(B)) < \infty. \quad \blacksquare$$

To close this section, we show that the partial trace of the semi-group difference of DD^* and D^*D is trace-class.

Proposition 2.29. *Let B satisfy Hypothesis 2.12, and let $t > 0$. Then, $\text{tr}_{\mathbb{C}^r}(e^{-tD_B^*D_B} - e^{-tD_BD_B^*}) \in S^1(L^2(\mathbb{R}^d, H))$.*

Proof. Let $C > 0$ be large enough, and let $\rho \in (0, \frac{\pi}{2})$ be small enough. Let $\Gamma := \Gamma_- \circ \Gamma_+^{-1}$, where $\Gamma_\pm(s) := -C \pm e^{i\rho}s$, $s \in [0, \infty)$, and $\circ, ^{-1}$ denote the composition of paths, respectively, the reversal of a path. Note that Γ encloses the non-negative real axis once. Then, for $\lambda \geq 0$, we have by Cauchy's integral formula

$$e^{-t\lambda} = \partial_\lambda^{N-1}((-t)^{1-N} e^{-t\lambda}) = \frac{(N-1)!(-t)^{1-N}}{2\pi i} \int_\Gamma \frac{e^{-tz}}{(z-\lambda)^N} dz.$$

Via holomorphic functional calculus, we, thus, have

$$\begin{aligned} e^{-tD_B^*D_B} - e^{-tD_B D_B^*} \\ = \frac{(N-1)!(-t)^{1-N}}{2\pi i} \int_{\Gamma} e^{-tz} (R_{-z}(D_B D_B^*)^N - R_{-z}(D_B^* D_B)^N) dz, \end{aligned}$$

where the integral exists as a Bochner integral in $B(L^2(\mathbb{C}^r \otimes H))$ in the norm topology. Therefore, we may interchange $\mathrm{tr}_{\mathbb{C}^r}$ and integration to obtain

$$\begin{aligned} \mathrm{tr}_{\mathbb{C}^r} (e^{-tD_B^*D_B} - e^{-tD_B D_B^*}) \\ = \frac{(N-1)!(-t)^{1-N}}{2\pi i} \int_{\Gamma} e^{-tz} \mathrm{tr}_{\mathbb{C}^r} (R_{-z}(D_B D_B^*)^N - R_{-z}(D_B^* D_B)^N) dz. \quad (36) \end{aligned}$$

We claim that the right-hand side of (36) converges even as a Bochner integral in $S^1(L^2(\mathbb{R}^d, H))$. Indeed, by Proposition 2.28, we have some constant C' , such that we may estimate the integrand by

$$\begin{aligned} \|e^{-tz} \mathrm{tr}_{\mathbb{C}^r} (R_{-z}(DD^*)^N - R_{-z}(D^*D)^N)\|_{S^1(L^2(\mathbb{R}^d, H))} \\ \leq C' e^{-t(-C+\cos(\rho)|s|)}, \quad z = \Gamma(s), \end{aligned} \quad (37)$$

which is integrable over $s \in \mathbb{R}$. ■

3. Approximation of the operator function B

The goal of this section is to construct an approximating sequence $B_{\bullet}$ of the operator function B , which enables us to calculate the principal trace in the following sections. We remark that a similar but simpler approximation argument has been used as a standard technique, for example, in [24, 31] with the same goal. In the multidimensional setup in this paper, we unfortunately need a more elaborate approximation procedure caused by the requirement that $\nabla B_{\bullet}$ should be sufficiently smooth and trace-class valued, a fact which comes for free in the one-dimensional case. Before we proceed with an approximation statement, we present the following convolution result which grants us smoothing of the operator family without destroying its decay properties.

Definition 3.1. Let $O(d)$ be the orthogonal group in dimension d with (bi-invariant) Haar measure m , and let $(g_n)_{n \in \mathbb{N}} \subset C^\infty(O(d))$ be a delta sequence with supports decreasing to $\{\mathbb{1}\}$ of $O(d)$ with respect to the convolution given by the Haar measure.³

³Since $O(d)$ is a smooth Lie group, the usual construction of approximate units in $L^1(G)$ of locally compact groups (cf. [21, Chapter 13.2]) can be refined to be smooth.

For $\psi^d \in C_c^\infty(\mathbb{R}^d)$ non-negative with $\int_{\mathbb{R}} \psi(x) dx = 1$, let $\psi_n^d(x) := n^d \psi^d(nx)$ be the associated delta sequence of $\mathbb{R}^d$. Let $\phi \in C_c^\infty(\mathbb{R}^d)$ with $\phi \equiv 1$ near 0. For $\varepsilon > 0$, let

$$\mathcal{F}_\varepsilon := \{f \in C^1(\mathbb{R}^d, \mathbb{C}^{k \times k}) \mid \|f\|_{\mathcal{F}_\varepsilon} < \infty\},$$

$$\|f\|_{\mathcal{F}_\varepsilon} := \|f\|_{L^\infty} + \|\langle X \rangle \nabla f\|_{L^\infty} + \|\langle X \rangle^{1+\varepsilon} \partial_R f\|_{L^\infty}.$$

For $f \in \mathcal{F}_\varepsilon$, define

$$\begin{aligned} \delta_n(f)(x) &:= \phi(x) \int_{\mathbb{R}^d} \psi_n^d(x-y) f(y) dy \\ &+ (1 - \phi(x)) \int_0^\infty \int_{O(d)} \psi_n^1(\log r) g_n(Y) f(r^{-1} Y^* x) dm(Y) \frac{dr}{r}. \end{aligned} \quad (38)$$

Lemma 3.2. *For $\varepsilon > 0$, the operator family δ_n is uniformly bounded in $\mathcal{F}_\varepsilon$, and $\delta_n(f)$, respectively, $\nabla \delta_n(f)$ converge point-wise to f , respectively, ∇f . For $f \in \mathcal{F}_\varepsilon$, the function $\delta_n(f)$ is smooth with bounded derivatives for all $n \in \mathbb{N}$.*

Proof. Let $f_n := \delta_n(f)$. For $x_0 \in \mathbb{R}^d \setminus \{0\}$, extend

$$e_1 := \frac{x_0}{|x_0|}$$

to an orthonormal basis $(e_i)_{i=1}^d$ of $\mathbb{R}^d$. For a neighbourhood U of x_0 small enough, the vectors $(\frac{x}{|x|}, e_2, \dots, e_d)$, $x \in U$, are still a basis of $\mathbb{R}^d$. Denote by $O_U(x) := \text{GS}(\frac{x}{|x|}, e_2, \dots, e_d) \in O(d)$ the Gram–Schmidt procedure applied to this basis. The map O_U is smooth on U and thus for $x \in U$, using the symmetry of convolution,

$$\begin{aligned} &\int_0^\infty \int_{O_d} \psi_n^1(\log r) g_n(Y) f(r^{-1} Y^* x) dm(Y) \frac{dr}{r} \\ &= \int_0^\infty \int_{O(d)} \psi_n^1\left(\log \frac{|x|}{r}\right) g_n(O_U(x) Y^*) f(r Y_1) dm(Y) \frac{dr}{r}, \end{aligned} \quad (39)$$

where Y_1 denotes the first column of Y . Thus, (39) is smooth in x on U . Since $1 - \phi$ cuts away 0, we conclude that f_n is smooth, because all other components of (38) are clearly smooth. Since ψ_n^d and ϕ are compactly supported, $1 - \phi$ is supported away from 0 and ψ_n^1 is again compactly supported, one easily concludes, by standard estimates on the integrals, that all derivatives of f_n are bounded. It is also apparent that f_n and ∇f_n converge point-wise to f , respectively, ∇f , since for each point, due to the compact support of the Dirac sequences, the integrals in (38) can be changed to take place over compact sets, on which f and ∇f are uniformly continuous. It remains to check that there is a constant C such that $\|f_n\|_{\mathcal{F}_\varepsilon} \leq C$. Clearly, $|f_n(x)| \leq \|f\|_{L^\infty(\mathbb{R}^d)}$ for all $x \in \mathbb{R}^d$. Since ϕ is compactly supported, it is also clear that there is a constant C only dependent on ϕ and $s \geq 0$ such that

$$\|\langle X \rangle^s \nabla(\phi \cdot (\psi_n^d *_{\mathbb{R}^d} f))\|_{L^\infty(\mathbb{R}^d)} \leq C(\|f\|_{L^\infty(\mathbb{R}^d)} + \|\nabla f\|_{L^\infty(\mathbb{R}^d)}).$$

For the second summand of (38), note that if a derivative is applied to $1 - \phi$, we obtain a compactly supported function, hence a similar arbitrary decay result as for the first summand shown above. Differentiation of $f(r^{-1}Y^*x)$ yields

$$\begin{aligned}\partial_{x^i} f(r^{-1}Y^*x) &= r^{-1} \left\langle (\nabla f) \left(Y^* \frac{x}{r} \right), Y_i \right\rangle, \\ \partial_R f(r^{-1}Y^*x) &= r^{-1} (\partial_R f)(r^{-1}Y^*x),\end{aligned}$$

which implies for $f \in \mathcal{F}_\varepsilon$, and $x \in \text{supp}(1 - \phi)$,

$$\left| \langle x \rangle \partial_{x^i} \int_0^\infty \int_{O(d)} \psi_n^1(\log r) g_n(Y) f(r^{-1}Y^*x) dm(Y) \frac{dr}{r} \right| \leq C \|f\|_{\mathcal{F}_\varepsilon},$$

where C only depends on ϕ . Similarly, there are constants C' , C'' independent of f and n , such that, for $f \in \mathcal{F}_\varepsilon$, and $x \in \text{supp}(1 - \phi)$,

$$\begin{aligned}& \left| \langle x \rangle^{1+\varepsilon} \partial_R \int_0^\infty \int_{O(d)} \psi_n^1(\log r) g_n(Y) f(r^{-1}Y^*x) dm(Y) \frac{dr}{r} \right| \\ & \leq C' \|f\|_{\mathcal{F}_\varepsilon} \int_0^\infty \psi_n^1(\log r) r^\varepsilon \frac{dr}{r} \\ & = C' \|f\|_{\mathcal{F}_\varepsilon} \int_{\mathbb{R}} \psi^1(s) e^{n^{-1}\varepsilon s} ds \leq C'' \|f\|_{\mathcal{F}_\varepsilon}.\end{aligned}$$

We conclude that $\|f_n\|_{\mathcal{F}_\varepsilon}$ is uniformly bounded. ■

We now arrive at the central result of this section. The operator family B is approximated by a sequence of finite-rank valued operator families with improved regularity. In spirit, this statement is close to the approximation argument used, for example, in [24, 31] in the one-dimensional case.

Proposition and Definition 3.3. *Denote*

$$P_n := \mathbb{1}_{[-n, n]}(A_0), \quad n \in \mathbb{N}.$$

Let $(\phi_n)_{n \in \mathbb{N}} \subset \mathcal{D}$ be an orthonormal basis of H , and let K_n be the finite rank projection onto $\text{span}\{(\phi_j)_{j=1}^n\}$ in H for $n \in \mathbb{N}$. Identify the range of K_n with $\mathbb{C}^n$ and let δ_l be the mollification operator defined in Definition 3.1 with a fixed choice of cut-off functions and delta sequences.

Define for B satisfying Hypothesis 2.12,

$$\begin{aligned}B_n(x) &:= P_n B(x) P_n, \\ B_{n,m}(x) &:= K_m B_n(x) K_m, \\ B_{n,m,l} &:= \delta_l(B_{n,m}), \quad n, m, l \in \mathbb{N}.\end{aligned}$$

Then, there are constants C , C_n , and $C_{n,m}$, where C is universal, C_n is independent of m , and $C_{n,m}$ is independent of l , such that

$$\begin{aligned} \lim_{n \rightarrow \infty} \operatorname{tr}_{\mathbb{C}^r} (R_z(D_{B_n}^* D_{B_n})^N - R_z(D_{B_n} D_{B_n}^*)^N) \\ = \operatorname{tr}_{\mathbb{C}^r} (R_z(D_B^* D_B)^N - R_z(D_B D_B^*)^N), \end{aligned}$$

for $z \in \mathcal{D}_C(B)$,

$$\begin{aligned} \lim_{m \rightarrow \infty} \operatorname{tr}_{\mathbb{C}^r} (R_z(D_{B_{n,m}}^* D_{B_{n,m}})^N - R_z(D_{B_{n,m}} D_{B_{n,m}}^*)^N) \\ = \operatorname{tr}_{\mathbb{C}^r} (R_z(D_{B_n}^* D_{B_n})^N - R_z(D_{B_n} D_{B_n}^*)^N), \end{aligned}$$

for $\operatorname{dist}(z, (-\infty, 0]) \geq C_n$, and

$$\begin{aligned} \lim_{l \rightarrow \infty} \operatorname{tr}_{\mathbb{C}^r} (R_z(D_{B_{n,m,l}}^* D_{B_{n,m,l}})^N - R_z(D_{B_{n,m,l}} D_{B_{n,m,l}}^*)^N) \\ = \operatorname{tr}_{\mathbb{C}^r} (R_z(D_{B_{n,m}}^* D_{B_{n,m}})^N - R_z(D_{B_{n,m}} D_{B_{n,m}}^*)^N), \end{aligned}$$

for $\operatorname{dist}(z, (-\infty, 0]) \geq C_{n,m}$, are limits in $S^1(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$.

Proof. We start with

$$\begin{aligned} \lim_{n \rightarrow \infty} \operatorname{tr}_{\mathbb{C}^r} (R_z(D_{B_n}^* D_{B_n})^N - R_z(D_{B_n} D_{B_n}^*)^N) \\ = \operatorname{tr}_{\mathbb{C}^r} (R_z(D_B^* D_B)^N - R_z(D_B D_B^*)^N). \end{aligned} \quad (40)$$

We expand both sides of (40), according to the decomposition described in Proposition 2.28, into a finite sum of trace-class operators. Each summand consists (up to a constant scalar factor and possibly up to a constant bounded operator $\langle \not\partial \rangle^{-1} \langle X \rangle^{k\xi} L \langle X \rangle^{(d-k)\xi}$) of a product of operators with factors $u_z^\bullet(B_n)$, $V^\bullet(B_n)$, $i(\not\partial B_n) \langle M_0 \rangle^{-1}$, and $\langle M_0 \rangle (R_z(D_{B_n}^* D_{B_n})^k + R_z(D_{B_n} D_{B_n}^*)^k)$ with upper indices independent of n and B (suppressed here by $\bullet$), respectively, the same factors with B_n replaced by B . We first note that, since P_n commutes with A_0 and have norm 1,

$$\sup_{n \in \mathbb{N}} (\rho_z^{-2N}(B_n) + \rho_z^{2N}(B_n)) \leq \rho_z^{-2N}(B) + \rho_z^{2N}(B) \xrightarrow{\operatorname{dist}(z, (-\infty, 0]) \rightarrow \infty} 0,$$

and because P_n converges strongly to $\mathbb{1}_H$ for $n \rightarrow \infty$, we also have for any $\beta \in [-2N, 2N]$, and a.e. $x \in \mathbb{R}^d$, strong operator convergences in H of

$$\langle A_0 \rangle^\beta (B_n(x) + A_0)^2 \langle A_0 \rangle^{-2-\beta} \xrightarrow{n \rightarrow \infty} \langle A_0 \rangle^\beta (B(x) + A_0)^2 \langle A_0 \rangle^{-2-\beta},$$

and of

$$\langle A_0 \rangle^\beta \partial_i B_n(x) \langle A_0 \rangle^{-2-\beta} \xrightarrow{n \rightarrow \infty} \langle A_0 \rangle^\beta \partial_i B(x) \langle A_0 \rangle^{-2-\beta}, \quad i \in \{1, \dots, d\}.$$

The prerequisites of Lemma 2.21 are satisfied, such that we have SOTA convergences of all factors $\overline{u_z^\bullet(B_n)}$ to $\overline{u_z^\bullet(B)}$, and of

$$\begin{aligned} & \langle M_0 \rangle (R_z(D_{B_n}^* D_{B_n})^k + R_z(D_{B_n} D_{B_n}^*)^k) \\ & \xrightarrow{n \rightarrow \infty} \langle M_0 \rangle (R_z(D_B^* D_B)^k + R_z(D_B D_B^*)^k). \end{aligned}$$

Clearly, the same argument also implies SOTA convergence of $i(\not{D} B_n) \langle M_0 \rangle^{-1}$ to $i(\not{D} B) \langle M_0 \rangle^{-1}$. It remains to discuss the $S^d(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ -valued, respectively, $S^{d+1}(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ -valued operators $\overline{V^\bullet(B_n)}$. Since P_n commutes with A_0 and is constant on $\mathbb{R}^d$, we have $V^\bullet(B_n) = \tilde{P}_n V^\bullet(B) \tilde{P}_n$ with $\tilde{P}_n := \mathbb{1}_{L^2(\mathbb{R}^d, \mathbb{C}^r)} \otimes P_n$ which converges in SOTA to $\mathbb{1}_{L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)}$. Lemma 2.19, thus, implies that $\overline{V^\bullet(B_n)}$ converges in $S^d(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$, respectively, $S^{d+1}(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$, to $\overline{V^\bullet(B)}$. We conclude that (40) converges in trace-class by Lemma 2.19 for $z \in \mathcal{D}_C(B)$ for some universal constant C .

For the second step, we fix $n \in \mathbb{N}$, and consider the statement

$$\begin{aligned} & \lim_{m \rightarrow \infty} \operatorname{tr}_{\mathbb{C}^r} (R_z(D_{B_{n,m}}^* D_{B_{n,m}})^N - R_z(D_{B_{n,m}} D_{B_{n,m}}^*)^N) \\ & = \operatorname{tr}_{\mathbb{C}^r} (R_z(D_{B_n}^* D_{B_n})^N - R_z(D_{B_n} D_{B_n}^*)^N). \end{aligned} \quad (41)$$

Note that we may not proceed analogously to the first step, since K_m , in contrast to P_n , does not necessarily commute with A_0 . However, since $\langle M_0 \rangle^s P_n$ is a bounded operator for all $s \in \mathbb{R}$, $n \in \mathbb{N}$, we note for B_n the stronger condition below holds:

$$\begin{aligned} & \tau^{0,0,\nabla,d,1}(B_n) < \infty, \\ & \exists \varepsilon > 0 : \tau^{0,0,\partial_R,d,1+\varepsilon}(B_n) < \infty. \end{aligned}$$

This allows us to simplify the decomposition in Proposition 2.28 to set $\alpha = 0$ and $\beta = 0$ in all appearing indices. In particular, no factor of the decomposition contains a function of M_0 . We suppress the new choice of indices by denoting them with $\tilde{\bullet}$. The same decomposition can be deployed for $B_{n,m}$ instead of B_n . Moreover, there exists $\eta > 0$ uniformly in m , and an m independent constant C such that

$$\tau^{0,0,\nabla,d,1}(B_{n,m}) + \tau^{0,0,\partial_R,d,1+\eta}(B_{n,m}) \leq C < \infty.$$

Since K_m is constant on $\mathbb{R}^d$, we have $V^{\tilde{\bullet}}(B_{n,m}) = \widetilde{K_m} V^{\tilde{\bullet}}(B_n) \widetilde{K_m}$, where the self-adjoint $\widetilde{K_m} := \mathbb{1}_{L^2(\mathbb{R}^d, \mathbb{C}^r)} \otimes K_m$ converge in strong operator topology to $\mathbb{1}_{L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H)}$. Thus, Lemmas 2.19 and 2.24 imply that $V^{\tilde{\bullet}}(B_{n,m})$ converges in d -th, respectively, $(d+1)$ -th Schatten–von Neumann norm to the operators $V^{\tilde{\bullet}}(B_n)$ as $m \rightarrow \infty$. Since $\|B_{n,m}\|_{C_b^1(\mathbb{R}^d, B(H))}$, $\|B_n\|_{C_b^1(\mathbb{R}^d, B(H))}$ are uniformly bounded in m , Lemma 2.22 implies that all factors $\overline{u_z^{\tilde{\bullet}}(B_{n,m})}$ converge in strong operator topology to $\overline{u_z^{\tilde{\bullet}}(B_n)}$, and that the last factor of type $\overline{u_z^{\tilde{\bullet}}(B_{n,m})}$ in each product of the decomposition converges

even in SOTA (because they do not involve $\not\partial$). Similarly, also $R_z(D_{B_{n,m}}^* D_{B_{n,m}})^k + R_z(D_{B_{n,m}} D_{B_{n,m}}^*)^k$ converges in SOTA to $R_z(D_{B_n}^* D_{B_n})^k + R_z(D_{B_n} D_{B_n}^*)^k$. The domain of convergence for the parameter z is uniformly given by

$$w = \text{dist}(z, (-\infty, 0]) \geq C,$$

for some constant C independent of m , according to Lemma 2.18, since the norm $\|B_{n,m}\|_{C_b^1(\mathbb{R}^d, B(H))}$ is uniformly bounded in m . Clearly, also, $i(\not\partial B_{n,m})$ converges in SOTA to $i\not\partial^E B_n$. We conclude that (41) converges in trace class for $w \geq C$ for some m -independent constant C by Lemma 2.19.

For the third step, fix both $n, m \in \mathbb{N}$, and consider the statement

$$\begin{aligned} & \lim_{l \rightarrow \infty} \text{tr}_{\mathbb{C}^r} (R_z(D_{B_{n,m,l}}^* D_{B_{n,m,l}})^N - R_z(D_{B_{n,m,l}} D_{B_{n,m,l}}^*)^N) \\ &= \text{tr}_{\mathbb{C}^r} (R_z(D_{B_{n,m}}^* D_{B_{n,m}})^N - R_z(D_{B_{n,m}} D_{B_{n,m}}^*)^N). \end{aligned} \quad (42)$$

First, note that $B_{n,m}(x) = K_m B_{n,m}(x) K_m$, and thus, also,

$$B_{n,m,l}(x) = K_m B_{n,m,l}(x) K_m \quad \text{and} \quad \nabla B_{n,m,l}(x) = K_m \nabla B_{n,m,l}(x) K_m.$$

In particular, if we identify $\text{rg}(K_m) \simeq \mathbb{C}^m$, there is some l -independent $\eta > 0$ such that

$$\tau^{0,0,\nabla,d,1}(B_{n,m,l}) + \tau^{0,0,\partial_R,d,1+\eta}(B_{n,m,l}) \leq \|B_{n,m,l}\|_{\mathcal{F}_\varepsilon} \leq C < \infty.$$

Additionally, $B_{n,m,l}$ and $\nabla B_{n,m,l}$ converge point-wise to $B_{n,m}$ and $\nabla B_{n,m}$, respectively, by Lemma 3.2. We use the same decomposition with $\alpha = 0$ and $\beta = 0$ from the second step; then, Lemma 2.22 implies that all factors $\overline{u_z^\bullet(B_{n,m,l})}$ converge in strong operator topology to $\overline{u_z^\bullet(B_{n,m})}$, and that the last factor of type $\overline{u_z^\bullet(B_{n,m,l})}$ in each product of the decomposition converges even in SOTA. Similarly, also,

$$R_z(D_{B_{n,m,l}}^* D_{B_{n,m,l}})^k + R_z(D_{B_{n,m,l}} D_{B_{n,m,l}}^*)^k$$

converges in SOTA to

$$R_z(D_{B_{n,m}}^* D_{B_{n,m}})^k + R_z(D_{B_{n,m}} D_{B_{n,m}}^*)^k.$$

Clearly, also, $i(\not\partial B_{n,m,l})$ converges in SOTA to $i(\not\partial B_{n,m})$. The domain of convergence for the parameter z is uniformly given by $\text{dist}(z, (-\infty, 0]) \geq C$, for some constant C independent of l , according to Lemma 2.18, since $\|B_{n,m,l}\|_{C_b^1(\mathbb{R}^d, B(H))} \leq \|B_{n,m,l}\|_{\mathcal{F}_\varepsilon}$ is uniformly bounded in l by Lemma 3.2. Because K_m is finite rank, and $\nabla B_{n,m,l}$, respectively, $\partial_R B_{n,m,l}$, can be bounded in S^d -norm by multiples of $\langle X \rangle^{-1}$, respectively, of $\langle X \rangle^{-1-\varepsilon}$ uniformly in l , the dominated convergence theorem and

Corollary 2.9 imply that the factors $V^{\tilde{}}(B_{n,m,l})$ converge in $S^d(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$, respectively, $S^{d+1}(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$. Together, we conclude that (42) converges in trace class for $w \geq C$ for some l -independent constant C by Lemma 2.19. ■

A simple consequence of holomorphic functional calculus and the possibility of choosing uniform integration paths allow us to conclude the approximation of the principal trace in its exponentiated form.

Corollary 3.4. *Let B satisfy Hypothesis 2.12, and let $t > 0$. Then, the iterated limits*

$$\begin{aligned} & \lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} \lim_{l \rightarrow \infty} \operatorname{tr}_{\mathbb{C}^r} (e^{-tD_{B_{n,m,l}}^*} D_{B_{n,m,l}} - e^{-tD_{B_{n,m,l}}} D_{B_{n,m,l}}^*) \\ &= \operatorname{tr}_{\mathbb{C}^r} (e^{-tD_B^*} D_B - e^{-tD_B} D_B^*) \end{aligned}$$

are limits in the trace norm of $L^2(\mathbb{R}^d, H)$.

Proof. According to Proposition and Definition 3.3, the trace norm bound from Proposition 2.28 holds uniformly in $n \in \mathbb{N}$ for B_n instead of B , on the domain

$$\operatorname{dist}(z, (-\infty, 0]) \geq C$$

for C independent of n . So, we may replace D_B and D_B^* with D_{B_n} and $D_{B_n}^*$ in equation (36) with the same integrable dominant (37), and the dominated convergence theorem allows us to pass the limit in trace norm past the integral in (36). In a similar fashion, we argue for the two iterated limits in m , respectively, l , where we might have to modify the integration curve dependent on n for the limit in m (respectively, dependent on n, m for the limit in l) in the proof of Proposition 2.29 accordingly. This is possible due to statement in Proposition and Definition 3.3 pertaining to the domains of convergence for the parameter z . ■

We present some properties of the approximating sequence $B_{n,m,l}$ in the upcoming remark, which closes this section on the approximation scheme.

Definition 3.5. For $l, s \in \mathbb{N}$, $p \in [1, \infty]$, and a Banach space X , denote by $C^{l,p}(\mathbb{R}^s, X)$ the space of l -times continuously differentiable functions with derivatives in L^p over $\mathbb{R}^d$ with values in X . For $l, m, n, s \in \mathbb{N}_0$ with $m \geq n$, denote the Banach space,

$$C_{m,n}^l(\mathbb{R}^s) := C^{l,\infty}(\mathbb{R}^s, B(\mathbb{C}^r) \otimes \langle A_0 \rangle^{-m} B(H) \langle A_0 \rangle^n),$$

with the norm

$$\|f\|_{l,m,n} := \sum_{\alpha \in \mathbb{N}_0^s, |\alpha| \leq l} \|\partial^\alpha f\|_{L^\infty(\mathbb{R}^d, B(\mathbb{C}^r) \otimes \langle A_0 \rangle^{-m} B(H) \langle A_0 \rangle^n)}, \quad f \in C_{m,n}^l(\mathbb{R}^s).$$

Let $C_{m,n}^{l,S^1}(\mathbb{R}^s)$ denote the Banach space $C^{l,p}(\mathbb{R}^s, B(\mathbb{C}^r) \otimes \langle A_0 \rangle^{-m} S^1(H) \langle A_0 \rangle^n)$ with the norm

$$\|f\|_{l,m,n}^{S^1} := \sum_{\alpha \in \mathbb{N}_0^s, |\alpha| \leq l} \|\partial^\alpha f\|_{L^\infty(\mathbb{R}^d, B(\mathbb{C}^r) \otimes \langle A_0 \rangle^{-m} S^1(H) \langle A_0 \rangle^n)}, \quad f \in C_{m,n}^{l,S^1}(\mathbb{R}^s).$$

Remark 3.6. Assume that B satisfies Hypothesis 2.12.

- (1) By (16) for $\phi \in \text{Dom } A_0$, a.e. $y \in S_1(0)$, a.e. $x \in \mathbb{R}^d$, and $\gamma \in \mathbb{N}_0^d$ with $|\gamma| \leq 1$, we have

$$\lim_{R \rightarrow \infty} R^{|\gamma|} \|(\partial^\gamma B(Ry + x) - \partial^\gamma B(Ry))\phi\|_H = 0.$$

Then, for a.e. $y \in S_1(0)$, a.e. $x \in \mathbb{R}^d$, and $\gamma \in \mathbb{N}_0^d$ with $|\gamma| \leq 1$, we have

$$\lim_{R \rightarrow \infty} R^{|\gamma|} \|\partial^\gamma B_{n,m,l}(Ry + x) - \partial^\gamma B_{n,m,l}(Ry)\|_{\langle A_0 \rangle^{-i} S^1(H) \langle A_0 \rangle^j} = 0$$

for all $n, m, l \in \mathbb{N}$, $i, j \in \mathbb{N}_0$.

- (2) Similarly, the third set of conditions of Hypothesis 2.12 imply that, for a.e. $y \in S_1(0)$, $z' \in \mathbb{R}^d$, and for $c > 0$, we have

$$\sup_{|x| \geq 1} |x|^{\frac{1}{2}} \sup_{z \in B_{c \log |x|}(0)} \|B_{n,m,l}(x + z) - B_{n,m,l}(x)\|_{\langle A_0 \rangle^{-i} S^1(H) \langle A_0 \rangle^j} < \infty, \quad (43)$$

$$\begin{aligned} & \sup_{|x| \geq 1} |x| \sup_{z \in B_{c \log |x|}(0)} \|w_z^2(B_{n,m,l})(x)\|_{\langle A_0 \rangle^{-i} S^1(H) \langle A_0 \rangle^j} < \infty, \\ & \sup_{|x| \geq 1} |x|^{\frac{3}{2}} \sup_{z \in B_{c \log |x|}(0)} m_d(z) \|\nabla B_{n,m,l}(x + z) \\ & \quad - \nabla B_{n,m,l}(x)\|_{\langle A_0 \rangle^{-i} S^1(H) \langle A_0 \rangle^j} < \infty, \end{aligned} \quad (44)$$

$$\sup_{|x| \geq 1} |x|^2 \sup_{z \in B_{c \log |x|}(0)} m_d(z) \|w_z^2(\nabla B_{n,m,l})(x)\|_{\langle A_0 \rangle^{-i} S^1(H) \langle A_0 \rangle^j} < \infty, \quad (45)$$

$$\lim_{R \rightarrow \infty} R \|w_{z'}^2(B_{n,m,l})(Ry)\|_{\langle A_0 \rangle^{-i} S^1(H) \langle A_0 \rangle^j} = 0, \quad (46)$$

$$\lim_{R \rightarrow \infty} R^2 \|w_{z'}^2(\nabla B_{n,m,l})(Ry)\|_{\langle A_0 \rangle^{-i} S^1(H) \langle A_0 \rangle^j} = 0, \quad (47)$$

for all $n, m, l \in \mathbb{N}$, $i, j \in \mathbb{N}_0$.

- (3) For all $n, m, l \in \mathbb{N}$, $i, j \in \mathbb{N}_0$, we have

$$(B_{n,m,l} + M_0)^2 - M_0^2, \quad i(\not\partial B_{n,m,l}) \in C_{i,j}^{\infty,S^1}(\mathbb{R}^d).$$

The projection P_n commutes with A_0 and K_m is finite rank, which maps into any $\text{Dom } A_0^i$, $i \in \mathbb{N}_0$; thus, the first and second statements hold for $B_{n,m}$ instead of $B_{n,m,l}$. But then $B_{n,m,l} = \delta_l(B_{n,m})$, which together with the dominated convergence theorem

(amenable since $\|B_{n,m}\|_{\mathcal{F}_\varepsilon} < \infty$ for some $\varepsilon > 0$) yields the first statement. The second statement is true for similar reasons; in particular, only large $|x|$ behaviour matters, which simplifies δ_l to be given purely by the radially symmetric convolution. Then, one exploits the radial symmetry of the conditions in the third set of conditions in Hypothesis 2.12. The third statement follows again since P_n commutes with A_0 and K_m is finite rank, mapping into any $\text{Dom } A_0^i$, $i \in \mathbb{N}_0$, and because the range of δ_l is smooth by Lemma 3.2.

4. Construction of auxiliary integral kernels related to the semi-groups of D^*D and DD^*

The overarching goal of this and the following sections is to calculate the principal trace. Since we assume Hypothesis 2.12 for B , we may facilitate this task, by replacing B by $B_{n,m,l}$ (and D_B , D_B^* by $D_{B_{n,m,l}}$, $D_{B_{n,m,l}}^*$ accordingly), Corollary 3.4 enables us to then take the iterated limits in the end to obtain the desired result. For convenience of notation, in the bulk of this and the following sections, we drop the indices n, m, l , which will be reintroduced at the end.

Let us first introduce some shorthand notations.

Definition 4.1. Denote by $\Delta_l \subset [0, 1]^l$ the l -simplex:

$$\Delta_l = \{w \in [0, 1]^l \mid w_l \leq w_{l-1} \leq \dots \leq w_1\}.$$

We will frequently use the following parametrization of Δ_l by $l + 1$ coordinates:

$$s_0 = 1 - w_1, \quad s_1 = w_1 - w_2, \dots, s_{l-1} = w_{l-1} - w_l, \quad s_l = w_l,$$

which satisfies $s_j \in [0, 1]$, and $\sum_{j=0}^l s_j = 1$. Note that $\text{vol}(\Delta_l) = \frac{1}{l!}$. Denote for a Hilbert space Y a self-adjoint operator T in Y , bounded below, and $s \in (\mathbb{R}^{\geq 0})^l$,

$$e^{-sT} := (e^{-s_1 T}, \dots, e^{-s_l T}) \in B(Y)^l,$$

and

$$T^{\otimes l} := (T, \dots, T) \in B(Y)^l.$$

Denote by $L^0(X, B)$ the measurable functions on a measure space X with values in a Banach space B . For $M \in L^0(X, B)$, denote

$$M^{\otimes l} := (M, \dots, M) \in (L^0(X, B))^l,$$

and for $s \in (\mathbb{R}^{\geq 0})^l$, $\mathbb{R}^{\geq 0} \ni t \mapsto N_t \in L^0(X, B)$,

$$N_s := (N_{s_1}, \dots, N_{s_l}) \in (L^0(X, B))^l.$$

Define the convolution shuffle product $\sqcup_*$ between $(L^0(\mathbb{R}^d \times \mathbb{R}^d, B(Y)))^{l+1}$ and $(L^0(\mathbb{R}^d, B(Y)))^l$ with values in $L^0(\mathbb{R}^d \times \mathbb{R}^d, B(Y))$ by

$$\begin{aligned}(q \sqcup_* M)(x, y) &:= \int_{u \in (\mathbb{R}^d)^l} q_0(x, u_1) M_1(u_1) q_1(u_1, u_2) \\ &\quad \cdots M_l(u_l) q_l(u_l, y) du \in B(Y), \\ q &= (q_0, \dots, q_l) \in (L^0(\mathbb{R}^d \times \mathbb{R}^d, B(Y)))^{l+1}, \\ M &= (M_1, \dots, M_l) \in (L^0(\mathbb{R}^d, B(Y)))^l,\end{aligned}$$

whenever the integral converges absolutely in $B(Y)$ -norm for a.e. $(x, y) \in \mathbb{R}^d \times \mathbb{R}^d$.

We want to calculate the trace of an operator in $L^2(\mathbb{R}^d, H)$, and thus, it is helpful to find a $B(H)$ -valued integral kernel and integrate its trace in H over the diagonal, which is intuitive, considering the scalar case covered by the well-known theorem by Mercer. A Hilbert space version is provided in the appendix of [11], albeit only for $\mathbb{R}^d$, $d = 1$. However, for general $d \in \mathbb{N}$, the original proof works with the necessary simple changes (which we omit here).

Theorem 4.2 ([11]). *Let Y be a separable Hilbert space, and $T \in S^1(L^2(\mathbb{R}^d, Y))$. Then, there exists a unique $S^1(Y)$ -valued measurable integral kernel t of T , such that*

$$(Tf)(x) = \int_{\mathbb{R}^d} t(x, y) f(y) dy, \quad f \in L^2(\mathbb{R}^d, Y),$$

and

$$h \mapsto (x \mapsto t(x, x + h))$$

is a bounded continuous map of $\mathbb{R}^d$ to $L^1(\mathbb{R}^d, S^1(Y))$. Moreover,

$$\begin{aligned}\int_{\mathbb{R}^d} \|t(x, x)\|_{S^1(Y)} dx &\leq \|T\|_{S^1(L^2(\mathbb{R}^d, Y))}, \\ \int_{\mathbb{R}^d} \operatorname{tr}_Y(t(x, x)) dx &= \operatorname{tr}_{L^2(\mathbb{R}^d, Y)}(T).\end{aligned}$$

Remark 4.3. We note that the variational principle and the separability of Y imply that if we find a jointly continuous $B(Y)$ -valued integral kernel $\tilde{t}$ of T , by the above stated uniqueness, we have already $t = \tilde{t}$ as elements of $C_b(\mathbb{R}^d, L^1(\mathbb{R}^d, S^1(Y)))$. Therefore, if we want to calculate the trace of T , it suffices to integrate the Y -trace of the diagonal of the continuous kernel of T , if it exists.

The next goal, therefore, is the construction of a continuous, $B(H)$ -valued integral kernel of $\operatorname{tr}_{\mathbb{C}^r}(e^{-tD^*D} - e^{-tDD^*})$. To that end, we will use a classical Volterra series argument.

Lemma 4.4. *Let T, S be self-adjoint operators in a Hilbert space Y , and assume that S is bounded with norm c , and $T \geq 0$. Then, for $t > 0$,*

$$e^{-t(T+S)} = e^{-tT} + \sum_{l=1}^{\infty} (-1)^l \int_{s \in t\Delta_l} e^{-sT} \sqcup S^{\otimes l} ds, \quad (48)$$

where sum and integral converge absolutely in operator norm.

Proof. Duhamel's principle implies, for $t > 0$,

$$e^{-t(T+S)} = e^{-tT} - \int_0^t e^{-(t-s)T} S e^{-s(T+S)} ds, \quad (49)$$

where the integral converges in operator norm. The iterative implementation of formula (49) then implies (48). It remains to show that (48) converges absolutely in operator norm. We estimate

$$\int_{s \in t\Delta_l} \|e^{-sT} \sqcup S^{\otimes l}\|_{B(Y)} ds \leq \frac{(ct)^l}{l!},$$

which is absolutely summable over $l \in \mathbb{N}$. ■

Definition 4.5. Let $t > 0, k \in \mathbb{N}$, and define

$$R_t^k := \begin{cases} e^{-tH_B}, & k = 0, \\ \int_{s \in t\Delta_k} e^{-sH_B} \sqcup (i\not{B})^{\otimes k} ds, & k \geq 1. \end{cases}$$

Since $i\not{B}^E B$ is a bounded operator, the integrals defining R_t^k converge absolutely in operator norm. We furthermore note that the norms of R_t^k are absolutely summable over $k \in \mathbb{N}$.

Lemma 4.6. *Let $t > 0$; then,*

$$\begin{aligned} e^{-tDD^*} &= \sum_{l=0}^{\infty} (-1)^l R_t^l, \\ e^{-tD^*D} &= \sum_{l=0}^{\infty} R_t^l, \end{aligned}$$

where the series converges absolutely in operator norm.

Proof. Apply Lemma 4.4 to

$$DD^* = H_B + i\not{B}B \quad \text{and} \quad D^*D = H_B - i\not{B}B. \quad \blacksquare$$

Definition 4.7. Let $t > 0, l \in \mathbb{N}$. We define

$$K_t^{-,l} := \sum_{j=\frac{l-1}{2}}^{\infty} R_t^{2j+1}, \quad l \text{ odd}, \quad K_t^{+,l} := \sum_{j=\frac{l}{2}}^{\infty} R_t^{2j}, \quad l \text{ even},$$

$$k_t^{-,l} := \sum_{j=0}^{\frac{l-3}{2}} R_t^{2j+1}, \quad l \text{ odd}, \quad k_t^{+,l} := \sum_{j=1}^{\frac{l-2}{2}} R_t^{2j}, \quad l \text{ even},$$

where the series converge in operator norm.

Lemma 4.6 then allows to re-express the semi-group difference in terms of commutators.

Lemma 4.8. Let $t > 0$; then,

$$\begin{aligned} e^{-tD^*D} - e^{-tDD^*} &= \int_0^t \frac{1}{2} ([D, D^* e^{-sDD^*}] - [D^*, D e^{-sD^*D}]) ds \\ &= \int_0^t \left(\left[i\not{D}, i\not{D} \frac{1}{2} (e^{-sD^*D} - e^{-sDD^*}) \right] - \left[A, A \frac{1}{2} (e^{-sD^*D} - e^{-sDD^*}) \right] \right. \\ &\quad \left. + \left[i\not{D}, A \frac{1}{2} (e^{-sD^*D} + e^{-sDD^*}) \right] - \left[A, i\not{D} \frac{1}{2} (e^{-sD^*D} + e^{-sDD^*}) \right] \right) ds \\ &= \int_0^t \left([i\not{D}, i\not{D} (K_s^{-,d-2} + k_s^{-,d-2})] - [A, A (K_s^{-,d} + k_s^{-,d})] \right. \\ &\quad \left. + [i\not{D}, A (K_s^{+,d-1} + k_s^{+,d-1} + e^{-sH_B})] \right. \\ &\quad \left. - [A, i\not{D} (K_s^{+,d-1} + k_s^{+,d-1} + e^{-sH_B})] \right) ds, \end{aligned} \quad (50)$$

where the integrals converge strongly on $\text{Dom } H_0$.

Proof. Since $D e^{-sD^*D} \supseteq e^{-sDD^*} D$, and $D^* e^{-sDD^*} \supseteq e^{-sD^*D} D^*$, $s > 0$, we have

$$\begin{aligned} \partial_s (e^{-sD^*D} - e^{-sDD^*}) &= DD^* e^{-sDD^*} - D^* D e^{-sD^*D} \\ &\supseteq \frac{1}{2} ([D, D^* e^{-sDD^*}] - [D^*, D e^{-sD^*D}]), \end{aligned}$$

which implies the first line. The second line follows by expanding

$$D = i\not{D} + A, \quad D^* = -i\not{D} + A,$$

and the third line by Lemma 4.6. ■

We exploit the fact that H_B commutes with the Clifford matrices c^j , and the above expansion reduces if we apply the partial trace $\text{tr}_{\mathbb{C}^r}$.

Lemma 4.9. *Let $t > 0$; then,*

$$\begin{aligned} \operatorname{tr}_{\mathbb{C}^r}(e^{-tD^*D} - e^{-tDD^*}) &= \int_0^t (\operatorname{tr}_{\mathbb{C}^r}([\mathbf{i}\not\partial, \mathbf{i}\not\partial K_s^{-,d-2} + AK_s^{+,d-1}]) \\ &\quad - [A, \operatorname{tr}_{\mathbb{C}^r}(AK_s^{-,d} + \mathbf{i}\not\partial K_s^{+,d-1})]) ds, \end{aligned} \quad (51)$$

where the right-hand side converges in operator norm of $L^2(\mathbb{R}^d, H)$.

Proof. We remind ourselves that $\operatorname{tr}_{\mathbb{C}^r} = \sum_{i=1}^r \langle \cdot, e^i \rangle_{\mathbb{C}^r}$, for any orthonormal basis $(e^i)_{i=1}^r$, which in particular implies that $\operatorname{tr}_{\mathbb{C}^r}$ is continuous from $B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))$ to $B(L^2(\mathbb{R}^d, H))$, both equipped with the weak operator/the strong operator/the norm topology. We consider the last line of equation (50) of Lemma 4.8 and restrict the integrand to $\operatorname{Dom} H_0 = \mathbb{C}^r \otimes X$, where

$$X = (H^2(\mathbb{R}^d, H) \cap L^2(\mathbb{R}^d, \operatorname{Dom} A_0))$$

is dense in $L^2(\mathbb{R}^d, H)$. Since the integral converges strongly on $\operatorname{Dom} H_0$, we may interchange $\operatorname{tr}_{\mathbb{C}^r}$ with integration. Also, we note that all summands in the last line of (50), which involve e^{-sH_B} or the operators $k_s^{\pm,j}$, contain at most $d-1$ Clifford matrices c^i as factors. We consider Definition 4.7, and otherwise the factors e^{-rH_B} , $r > 0$, and A , which commute with all Clifford matrices: we obtain, analogously to Lemma 2.1, that these terms vanish, if $\operatorname{tr}_{\mathbb{C}^r}$ is applied. So, (51) holds, at least on X . We may estimate for $k \geq d-2 \geq 1$, and $R, S \in \{\mathbf{i}\not\partial, A\}$, using the fact that $\mathbf{i}(\not\partial B)$ is a C_b^1 -family with bounded derivatives of finite-rank operators with range in $\operatorname{Dom} A_0$, and the defining integral of R_s^k ,

$$\|\overline{STR_s^k}\|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))}, \quad \|\overline{SR_s^k T}\|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))} \leq C' \frac{c^{k-1} s^{k-1}}{(k-1)!}, \quad (52)$$

where $c := \|\mathbf{i}(\not\partial B)\|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))}$, and C' is a suitable constant. In particular, the norms in (52) are absolutely summable over $k \geq d-2$, so we have

$$\|\overline{STK_s^j}\|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))}, \quad \|\overline{SK_s^j T}\|_{B(L^2(\mathbb{R}^d, \mathbb{C}^r \otimes H))} \leq C' \sum_{k=j-1}^{\infty} \frac{c^k s^k}{k!},$$

which is $O(s^{j-1})$ for s near 0, and in particular, we see that $\overline{STK_s^j}$ and $\overline{SK_s^j T}$ are Bochner integrable in operator norm on $s \in (0, t)$ for any $t > 0$. Since $e^{-tD^*D} - e^{-tDD^*}$ is also bounded, and $\operatorname{tr}_{\mathbb{C}^r}$ is a continuous operator, equation (51) holds by density of X in $L^2(\mathbb{R}^d, H)$, and the right-hand side of (51) converges in operator norm. ■

We introduce the following building blocks of the desired integral kernel.

Definition 4.10. Let $t > 0$. Denote, for $j \geq 1$,

$$\begin{aligned} q_t(x) &:= (4\pi t)^{-\frac{d}{2}} e^{-\frac{|x|^2}{4t}}, \quad x \in \mathbb{R}^d, \quad Q_t := \mathbb{1}_{C^r} \otimes e^{-tA_0^2} \otimes q_t, \\ \theta_t^j &:= \int_{s \in t\Delta_j} Q_s \sqcup_* (A^2 - M_0^2)^{\otimes j} ds, \quad \theta_t := Q_t + \sum_{j=1}^{\infty} (-1)^j \theta_t^j, \\ r_t^j &:= \int_{s \in t\Delta_j} \theta_s \sqcup_* (i\not{D}B)^{\otimes j} ds. \end{aligned}$$

Remark 4.11. In the following, we will use the convention that if a statement is made for $C_{m',n}^{l',(S^1)}$, it means that it holds both for $C_{m',n}^{l'}$, respectively, $C_{m',n}^{l',S^1}$, consistently in place of all $C_{m',n}^{l',(S^1)}$ appearing throughout the statement. If no other domain is specified, it will always be $\mathbb{R}^d$.

In the following part, we will successively construct integral kernels together with estimates, which we build up to arrive at the desired integral kernels needed to calculate the principal trace. The arguments in each step are quite similar; the techniques involved are classical (for example, cf. [6, Chapter 2]).

Lemma 4.12. Let $l, l', m, m', n, n' \in \mathbb{N}_0$ with $m' \geq m \geq n \geq n'$, and $l' \geq l$. For $t > 0$, define the linear operators $Q_t^{L/R}$, given by

$$\begin{aligned} (Q_t^L f)(x) &:= \int_{\mathbb{R}^d} Q_t(x, y) f(y) dy, \\ (Q_t^R f)(x) &:= \int_{\mathbb{R}^d} f(y) Q_t(x, y) dy, \quad f \in C_{m,n}^{l,(S^1)}(\mathbb{R}^d). \end{aligned}$$

Then, Q_t^L is continuous as a map to $C_{m',n}^{l',(S^1)}$, and Q_t^R is continuous as a map to $C_{m,n'}^{l',(S^1)}$, and we have a t -independent constant C , such that

$$\begin{aligned} \|Q_t^L\|_{B(C_{m,n}^{l,(S^1)}, C_{m',n}^{l',(S^1)})} &\leq C t^{-\frac{l'-l+m'-m}{2}}, \\ \|Q_t^R\|_{B(C_{m,n'}^{l,(S^1)}, C_{m,n}^{l',(S^1)})} &\leq C t^{-\frac{l'-l+n-n'}{2}}. \end{aligned} \tag{53}$$

Proof. Let $f \in C_{m,n}^{l,(S^1)}$, $\alpha \in \mathbb{N}_0^d$ with $|\alpha| \leq l'$. For $|\alpha| \leq l$, let $\beta = 0 \in \mathbb{N}_0^d$; otherwise, let $\beta \in \mathbb{N}_0^d$, such that $\alpha \geq \beta$, $|\beta| = l' - l$ and $|\alpha - \beta| = l$. Then,

$$\begin{aligned} &\langle A_0 \rangle^{m'} \partial^\alpha (Q_t^L f)(x) \langle A_0 \rangle^{-n} \\ &= \int_{\mathbb{R}^d} (\partial^\beta q_t)(x - y) \langle A_0 \rangle^{m'-m} e^{-tA_0^2} \langle A_0 \rangle^m (\partial^{\alpha-\beta} f)(y) \langle A_0 \rangle^{-n} dy, \\ &\langle A_0 \rangle^m \partial^\alpha (Q_t^R f)(x) \langle A_0 \rangle^{-n'} \\ &= \int_{\mathbb{R}^d} \langle A_0 \rangle^m (\partial^{\alpha-\beta} f)(y) \langle A_0 \rangle^{-n} \langle A_0 \rangle^{n-n'} e^{-tA_0^2} (\partial^\beta q_t)(x - y) dy. \end{aligned}$$

There are constants C_β, c_r , such that

$$\|\partial^\beta q_t\|_{L^1(\mathbb{R}^d)} \leq C_\beta t^{-\frac{|\beta|}{2}} \quad \text{and} \quad \|\langle A_0 \rangle^r e^{-tA_0^2}\|_{B(H)} \leq c_r t^{-\frac{r}{2}},$$

while

$$\begin{aligned} \|\langle A_0 \rangle^m (\partial^{\alpha-\beta} f) \langle A_0 \rangle^{-n}\|_{L^\infty(\mathbb{R}^d, B(H))} &\leq \|f\|_{l,m,n}, \\ \|\langle A_0 \rangle^m (\partial^{\alpha-\beta} f) \langle A_0 \rangle^{-n}\|_{L^\infty(\mathbb{R}^d, S^1(H))} &\leq \|f\|_{l,m,n}^{S^1}, \end{aligned}$$

and so, the claims follow. $\blacksquare$

Lemma 4.13. *Let $n \in \mathbb{N}_0$; then, there is a constant c , such that for $t > 0$, $j \in \mathbb{N}$,*

$$\begin{aligned} &\int_{s \in t\Delta_j} \|(Q_s \sqcup_* (A^2 - M_0^2)^{\otimes j})(x, y)\|_{B(\mathbb{C}^r \otimes \text{Dom } A_0^n)} ds \\ &\leq \frac{(ct)^j}{j!} q_t(x - y), \quad x, y \in \mathbb{R}^d. \end{aligned} \quad (54)$$

Let $l, l', m, m', n \in \mathbb{N}_0$ with $m' \geq m \geq n \geq n'$, and $l' \geq l$. For $t > 0$ and $j \in \mathbb{N}_0$, define the linear operators $\Theta_t^{j,L/R}$, given by

$$\begin{aligned} (\Theta_t^{j,L} f)(x) &:= \int_{\mathbb{R}^d} \theta_t^j(x, y) f(y) dy, \\ (\Theta_t^{j,R} f)(x) &:= \int_{\mathbb{R}^d} f(y) \theta_t^j(x, y) dy, \quad f \in C_{m,n}^{l,(S^1)}(\mathbb{R}^d). \end{aligned}$$

Then, $\Theta_t^{j,L}$ is continuous as a map to $C_{m',n}^{l',(S^1)}$, and $\Theta_t^{j,R}$ is continuous as a map to $C_{m,n'}^{l',(S^1)}$, and there is a constant C , independent of j and t , such that

$$\begin{aligned} \|\Theta_t^{j,L}\|_{B(C_{m,n}^{l,(S^1)}, C_{m',n}^{l',(S^1)})} & \\ \|\Theta_t^{j,R}\|_{B(C_{m,n}^{l,(S^1)}, C_{m,n'}^{l',(S^1)})} &\leq \frac{C^j}{\prod_{i=1}^j \max(1, i - \frac{l'-l}{2})} t^{j - \frac{l'-l}{2}}. \end{aligned}$$

Proof. We begin with the estimate of (54). Let

$$c = \sup_{x \in \mathbb{R}^d} \overline{\|A(x)^2 - A_0^2\|_{B(\mathbb{C}^r \otimes \text{Dom } A_0^n)}}.$$

We have, for $x, y \in \mathbb{R}^d$,

$$\begin{aligned} &\int_{s \in t\Delta_j} \|(Q_s \sqcup_* (A^2 - M_0^2)^{\otimes j})(x, y)\|_{B(\mathbb{C}^r \otimes \text{Dom } A_0^n)} ds \\ &\leq \int_{s \in t\Delta_j} (q_s \sqcup_* c^{\otimes j})(x, y) ds = \frac{(ct)^j}{j!} q_t(x - y). \end{aligned}$$

For the following parts of the proof, we, therefore, may interchange iterated integration freely. We show only the properties of $\Theta_t^{j,L}$; the proof for $\Theta_t^{j,R}$ is analogous. Let L_f denote the operator given by $(L_f g)(x) = (fg)(x)$; for $x \in \mathbb{R}^d$, $f \in C_{m',m}^{l',(\mathbb{S}^1)}$, and $g \in C_{m,n}^{l',(\mathbb{S}^1)}(\mathbb{R}^d)$, we have, by the Leibniz rule and the ideal property of S^1 , that

$$\|L_f\|_{B(C_{m,n}^{l',(\mathbb{S}^1)}, C_{m',n}^{l',(\mathbb{S}^1)})} \leq d^{l'} \|f\|_{C_{m',m}^{l'}}. \quad (55)$$

In particular, there is a constant c' such that

$$\|L_{\overline{A^2 - M_0^2}}\|_{B(C_{m,n}^{l',(\mathbb{S}^1)}, C_{m',n}^{l',(\mathbb{S}^1)})} \leq c' d^{l'}.$$

We proceed inductively with convention $\theta_t^0 = Q_t$. For $j = 0$, the statement is Lemma 4.12. Let C' be the constant given by (53), which is independent of j and t . For $j \geq 0$, we have

$$\theta_t^{j+1}(x, y) = \int_0^t \int_{\mathbb{R}^d} \theta_s^j(x, z) (A^2(z) - A_0^2) Q_{t-s}(y, z) dz ds, \quad x, y \in \mathbb{R}^d.$$

Thus, by (55), we have

$$\begin{aligned} & \|\Theta_t^{j+1,L}\|_{B(C_{m,n}^{l,(\mathbb{S}^1)}, C_{m',n}^{l',(\mathbb{S}^1)})} \\ & \leq c' d^{l'} \int_0^{\frac{t}{2}} \|\Theta_s^{j,L}\|_{B(C_{m',n}^{l',(\mathbb{S}^1)})} \|Q_{t-s}^L\|_{B(C_{m,n}^{l,(\mathbb{S}^1)}, C_{m',n}^{l',(\mathbb{S}^1)})} ds \\ & \quad + c' d^l \int_{\frac{t}{2}}^t \|\Theta_s^{j,L}\|_{B(C_{m',n}^{l,(\mathbb{S}^1)}, C_{m',n}^{l',(\mathbb{S}^1)})} \|Q_{t-s}^L\|_{B(C_{m,n}^{l,(\mathbb{S}^1)})} ds \\ & \leq c' C' d^{l'} \frac{C^j}{\prod_{i=1}^j \max(1, i - \frac{l'-l}{2})} \left(\int_0^{\frac{t}{2}} s^j (t-s)^{-\frac{l'-l}{2}} ds + \int_{\frac{t}{2}}^t s^{j-\frac{l'-l}{2}} ds \right) \\ & \leq c C' d^{l'} t^{j+1-\frac{l'-l}{2}} \frac{C^j}{\prod_{i=1}^j \max(1, i - \frac{l'-l}{2})} \frac{2^{2+\frac{l'-l}{2}}}{\max(1, j+1 - \frac{l'-l}{2})} \\ & \leq \frac{C^{j+1}}{\prod_{i=1}^{j+1} \max(1, i - \frac{l'-l}{2})} t^{j+1-\frac{l'-l}{2}}, \end{aligned}$$

which holds if we set $C := 2^{2+\frac{l'-l}{2}} c' C' d^{l'}$, which is independent of j and t . ■

Corollary 4.14. *Let $n \in \mathbb{N}_0$; then, there is a constant c , such that, for $t > 0$,*

$$\sum_{j=0}^{\infty} \|\theta_t^j(x, y)\|_{B(\mathbb{C}^r \otimes \text{Dom } A_0^B)} \leq e^{ct} q_t(x - y), \quad x, y \in \mathbb{R}^d. \quad (56)$$

Let $t > 0$. Let $l, l', m, m', n, n' \in \mathbb{N}_0$ with $m' \geq m \geq n \geq n'$, and $l' \geq l$. Define the linear operators $\Theta_t^{L/R}$, given by

$$\begin{aligned}(\Theta_t^L f)(x) &:= \int_{\mathbb{R}^d} \theta_t(x, y) f(y) dy, \\(\Theta_t^R f)(x) &:= \int_{\mathbb{R}^d} f(y) \theta_t(x, y) dy, \quad f \in C_{m,n}^{l,(S^1)}(\mathbb{R}^d).\end{aligned}$$

Then, Θ_t^L is continuous as a map to $C_{m',n}^{l',(S^1)}$, and Θ_t^R is continuous as a map to $C_{m,n'}^{l',(S^1)}$, and there is a continuous function h , such that

$$\begin{aligned}\|\Theta_t^L\|_{B(C_{m,n}^{l,(S^1)}, C_{m',n}^{l',(S^1)})} &= t^{-\frac{l'-l+m'-m}{2}} h(t), \\ \|\Theta_t^R\|_{B(C_{m,n}^{l,(S^1)}, C_{m,n'}^{l',(S^1)})} &= t^{-\frac{l'-l+n-n'}{2}} h(t).\end{aligned}$$

Proof. Inequality (56) follows from inequality (54) and enables us to exchange integration and summation in the following. We have for $f \in C_{m,n}^{l,(S^1)}(\mathbb{R}^d)$, by Lemmas 4.12 and 4.13,

$$\begin{aligned}\|\Theta_t^L f\|_{C_{m',n}^{l',(S^1)}} &= \left\| \int_{\mathbb{R}^d} \left(\sum_{j=0}^{\infty} (-1)^j \theta_t^j(\cdot, y) \right) f(y) dy \right\|_{C_{m',n}^{l',(S^1)}} \\ &= \left\| \sum_{j=0}^{\infty} (-1)^j \Theta_t^{j,L} f \right\|_{C_{m',n}^{l',(S^1)}} \\ &\leq C t^{-\frac{l'-l+m'-m}{2}} + t^{-\frac{l'-l}{2}} \left(\sum_{j=1}^{\infty} \frac{(Ct)^j}{\prod_{i=1}^j \max(1, i - \frac{l'-l}{2})} \right) \|f\|_{C_{m,n}^{l,(S^1)}} \\ &= h(t) t^{-\frac{l'-l+m'-m}{2}} \|f\|_{C_{m,n}^{l,(S^1)}}\end{aligned}$$

for some continuous function h . Θ_t^R can be treated analogously. $\blacksquare$

Lemma 4.15. Let $l, m, n \in \mathbb{N}_0$ with $m \geq n$. Then, there exists a constant C , such that, for $t > 0$, $j \in \mathbb{N}_0$,

$$\|\theta_t^j\|_{C_{m,n}^l(\mathbb{R}^{2d})} \leq \begin{cases} C t^{-\frac{l+m-n+d}{2}}, & j = 0, \\ \frac{C^j}{\prod_{i=1}^j \max(1, i - \frac{l+d}{2})} t^{j - \frac{l+d}{2}}, & j \geq 1. \end{cases}$$

Proof. We proceed inductively in j . For $j = 0$, the statement follows from

$$\|Q_t\|_{C_{m,n}^l(\mathbb{R}^{2d})} \leq \| \langle A_0 \rangle^{m-n} e^{-tA_0^2} \|_{B(H)} \|q_t\|_{C_b^l(\mathbb{R}^d)} \leq C' t^{-\frac{l+m-n+d}{2}},$$

where C' is some constant independent of t . Recall that there is a constant c , such that

$$\|L_{\overline{A^2-M_0^2}}\|_{B(C_{n,n}^l, C_{m,n}^l)} \leq cd^l.$$

Let R_f denote the operator $(R_f g)(x) := g(x)f(x)$. Then, similarly, we have

$$\|R_{\overline{A^2-M_0^2}}\|_{B(C_{n,n}^l, C_{m,n}^l)} \leq cd^l.$$

For $j \geq 0$, we have, for $x, y \in \mathbb{R}^d$,

$$\begin{aligned} \theta_t^{j+1}(x, y) &= \int_0^t \int_{\mathbb{R}^d} \theta_s^j(x, z) (A^2(z) - A_0^2) Q_{t-s}(y, z) dz ds, \\ &= \int_0^{\frac{t}{2}} \Theta_s^{j,L} ((A^2 - M_0^2) Q_{t-s}(\cdot, y))(x) ds \\ &\quad + \int_{\frac{t}{2}}^t Q_{t-s}^R (\theta_s^j(x, \cdot) (A^2 - M_0^2))(y) ds, \end{aligned} \quad (57)$$

and thus, we have constant C'' , independent of j and t , such that

$$\begin{aligned} \|\theta_t^{j+1}\|_{C_{m,n}^l(\mathbb{R}^{2d})} &\leq cd^l C' C'' \frac{C^j}{j!} \int_0^{\frac{t}{2}} s^j (t-s)^{-\frac{l+d}{2}} ds \\ &\quad + cd^l \frac{C^j}{\prod_{i=1}^j \max(1, i - \frac{l+d}{2})} \int_{\frac{t}{2}}^t s^{j-\frac{l+d}{2}} ds \\ &\leq \frac{C^{j+1}}{\prod_{i=1}^{j+1} \max(1, i - \frac{l+d}{2})} t^{j+1-\frac{l+d}{2}}, \end{aligned} \quad (58)$$

if we choose C , dependent on c, C', C'', l , large enough. $\blacksquare$

Corollary 4.16. *Let $l, m, n \in \mathbb{N}_0$ with $m \geq n$. Then, $\theta_t \in C_{m,n}^l(\mathbb{R}^{2d})$ for $t > 0$, and there is a continuous function h , such that*

$$\|\theta_t\|_{C_{m,n}^l(\mathbb{R}^{2d})} = h(t) t^{-\frac{l+m-n+d}{2}}, \quad t > 0.$$

Proof. We have

$$\begin{aligned} \|\theta_t\|_{C_{m,n}^l(\mathbb{R}^{2d})} &\leq \sum_{j=0}^{\infty} \|\theta_t^j\|_{C_{m,n}^l(\mathbb{R}^{2d})} \\ &\leq C t^{-\frac{l+m-n+d}{2}} + \left(\sum_{j=1}^{\infty} \frac{C^j}{\prod_{i=1}^j \max(1, i - \frac{l+d}{2})} t^j \right) t^{-\frac{l+d}{2}} \\ &=: h(t) t^{-\frac{l+m-n+d}{2}}. \end{aligned} \quad \blacksquare$$

Lemma 4.17. *Let $n \in \mathbb{N}_0$; then, there is a constant c , such that for $t > 0$, $j \in \mathbb{N}$, and $x, y \in \mathbb{R}^d$,*

$$\int_{s \in t \Delta_j} \|(\theta_s \lrcorner_* (i\rlap{/}\partial B)^{\otimes j})(x, y)\|_{B(\mathbb{C}^r) \otimes \langle A_0 \rangle^{-n} S^1(H) \langle A_0 \rangle^n} ds \leq \frac{(ct)^j}{j!} e^{ct} q_t(x - y).$$

Let $l, l', m, m', n \in \mathbb{N}_0$ with $m' \geq m \geq n \geq n'$, and $l' \geq l$. For $t > 0$ and $j \in \mathbb{N}$, define the linear operator $R_t^{j,L}$, given by

$$(R_t^{j,L} f)(x) := \int_{\mathbb{R}^d} r_t^j(x, y) f(y) dy, \quad f \in C_{m,n}^l(\mathbb{R}^d).$$

Then, $R_t^{j,L}$ is continuous as a map to $C_{m',n}^{l',S^1}$, and for $0 < t \leq t_0$, there exists a constant C , independent of $j \in \mathbb{N}$ and $t > 0$, such that

$$\|R_t^{j,L}\|_{B(C_{m,n}^l, C_{m',n}^{l',S^1})} \leq \frac{C^j}{\prod_{i=1}^j \max(1, i - \frac{l'-l}{2})} t^{j - \frac{l'-l}{2}}.$$

Proof. By (56), we have for $n \in \mathbb{N}_0$ a constant c' , such that, for $t > 0$,

$$\|\theta_t\|_{B(\mathbb{C}^r \otimes \text{Dom } A_0^n)} \leq e^{c't} q_t(x - y).$$

We recall that $(\rlap{/}\partial B)$ is finite rank valued and thus, with

$$c := \max(c', \sup_{x \in \mathbb{R}^d} \|i(\rlap{/}\partial B)\|_{B(\mathbb{C}^r) \otimes \langle A_0 \rangle^{-n} S^1(H) \langle A_0 \rangle^n}),$$

we have, for $x, y \in \mathbb{R}^d$,

$$\begin{aligned} & \int_{s \in t \Delta_j} \|(\theta_s \lrcorner_* (i\rlap{/}\partial B)^{\otimes j})(x, y)\|_{B(\mathbb{C}^r) \otimes \langle A_0 \rangle^{-n} S^1(H) \langle A_0 \rangle^n} ds \\ & \leq \int_{s \in t \Delta_j} (e^{cs} q_s \lrcorner_* c^{\otimes j})(x, y) ds = \frac{(ct)^j}{j!} e^{ct} q_t(x - y), \end{aligned}$$

and thus, we may exchange integration freely in the following. We note that there is a constant c , such that

$$\|L_{i(\rlap{/}\partial B)}\|_{B(C_{n,n}^l, C_{m,n}^{l,S^1})} + \|R_{i(\rlap{/}\partial B)}\|_{B(C_{m,m}^l, C_{m,n}^{l,S^1})} \leq cd^l.$$

With convention $r_t^0 := \theta_t$, $R_t^{0,L} := \Theta_t^L$, we have by Corollary 4.14, for $0 < t \leq t_0$, a constant C' , independent of t , such that

$$\|\Theta_t^L\|_{B(C_{m,n}^{l,(S^1)}, C_{m',n}^{l',(S^1)})} \leq C' t^{-\frac{l'-l+m'-m}{2}},$$

and thus,

$$\begin{aligned}
& \|R_t^{j+1,L}\|_{B(C_{m,n}^l, C_{m',n}^{l',S^1})} \\
& \leq cd^{l'} \int_0^{\frac{t}{2}} \|R_s^{j,L}\|_{B(C_{m',n}^{l',S^1})} \|\Theta_{t-s}^L\|_{B(C_{m,n}^l, C_{m',n}^{l',S^1})} ds \\
& + cd^l \int_{\frac{t}{2}}^t \|R_s^{j,L}\|_{B(C_{m',n}^l, C_{m',n}^{l',S^1})} \|\Theta_{t-s}^L\|_{B(C_{m,n}^{l',S^1})} ds \\
& \leq cC'd^{l'} \frac{C^j}{\prod_{i=1}^j \max(1, i - \frac{l-l'}{2})} \left(\int_0^{\frac{t}{2}} s^j (t-s)^{-\frac{l'-l}{2}} ds + \int_{\frac{t}{2}}^t s^{j-\frac{l'-l}{2}} ds \right) \\
& \leq cC'd^{l'} t^{j+1-\frac{l'-l}{2}} \frac{C^j}{\prod_{i=1}^j \max(1, i - \frac{l'-l}{2})} \frac{2^{2+\frac{l'-l}{2}}}{\max(1, j+1 - \frac{l'-l}{2})} \\
& \leq \frac{C^{j+1}}{\prod_{i=1}^{j+1} \max(1, i - \frac{l'-l}{2})} t^{j+1-\frac{l'-l}{2}},
\end{aligned}$$

which holds if we set $C := 2^{2+\frac{l'-l}{2}} cC'd^{l'}$, which is independent of j and t . $\blacksquare$

Lemma 4.18. *Let $n \in \mathbb{N}_0$; then, there is a constant c , such that, for $t > 0$,*

$$\sum_{j=1}^{\infty} \|r_t^j(x, y)\|_{B(\mathbb{C}^r) \otimes \langle A_0 \rangle^{-n} S^1(H) \langle A_0 \rangle^n} \leq e^{ct} q_t(x - y), \quad x, y \in \mathbb{R}^d.$$

Let $l, m, n \in \mathbb{N}_0$ with $m \geq n$, $1 \geq l$. For $0 < t \leq t_0$, there exists a constant C , independent of t and $j \in \mathbb{N}$, such that

$$\|r_t^j\|_{C_{m,n}^{l,S^1}(\mathbb{R}^{2d})} \leq \frac{C^j}{\prod_{i=1}^j \max(1, i - \frac{l+d}{2})} t^{j-\frac{l+d}{2}}.$$

Proof. Let $0 < t \leq t_0$ and C' be a constant, independent of t , such that

$$\|\theta_t\|_{C_{m,n}^{l,S^1}(\mathbb{R}^{2d})} \leq C' t^{-\frac{l+m-n+d}{2}}.$$

Recall that there is a constant c , such that

$$\|L_i(\emptyset B)\|_{B(C_{n,n}^l, C_{m,n}^{l,S^1})} + \|R_i(\emptyset B)\|_{B(C_{m,m}^l, C_{m,n}^{l,S^1})} \leq cd^l.$$

We have for $j \geq 0$ with convention $r_t^0 := \theta_t$, and $x, y \in \mathbb{R}^d$,

$$r_t^{j+1}(x, y) = \int_0^{\frac{t}{2}} R_s^{j,L}((\emptyset B)\theta_{t-s}(\cdot, y))(x) ds + \int_{\frac{t}{2}}^t \Theta_{t-s}^R(r_s^j(x, \cdot)(\emptyset B))(y) ds,$$

and thus, we have a constant C'' independent of j and t , such that

$$\begin{aligned} \|r_t^{j+1}\|_{C_{m,n}^{l,S^1}(\mathbb{R}^{2d})} &\leq cd^l C' C'' \frac{C^j}{j!} \int_0^{\frac{t}{2}} s^j (t-s)^{-\frac{l+d}{2}} ds \\ &\quad + cd^l C'' \frac{C^j}{\prod_{i=1}^j \max(1, i - \frac{l+d}{2})} \int_{\frac{t}{2}}^t s^{j-\frac{l+d}{2}} ds \\ &\leq \frac{C^{j+1}}{\prod_{i=1}^{j+1} \max(1, i - \frac{l+d}{2})} t^{j+1-\frac{l+d}{2}}, \end{aligned}$$

if we choose C , dependent on c, C', C'', l , large enough. $\blacksquare$

5. Construction of the main integral kernels

With the auxiliary kernels constructed in the previous section, we may now proceed to construct the integral kernels of the operators appearing in Lemma 4.9, which involve commutators.

Definition 5.1. Let $t > 0, k \in \mathbb{N}$. Define

$$\kappa_t^{-,k} := \sum_{j=\frac{k-1}{2}}^{\infty} r_t^{2j+1}, \quad k \text{ odd}, \quad \kappa_t^{+,k} := \sum_{j=\frac{k}{2}}^{\infty} r_t^{2j}, \quad k \text{ even}.$$

Moreover, define for $\varepsilon, R > 0$, with $\not\partial_{x/y/1}$ denoting the application of $\not\partial$ to the x -variable/ y -variable/first variable, for $x, y \in \mathbb{R}^d$,

$$\begin{aligned} \rho_t^{\varepsilon,R}(x, y) &:= \mathbb{1}_{B_R(0)}(x) \mathbb{1}_{B_R(0)}(y) \operatorname{tr}_{\mathbb{C}^r} (i(\not\partial_x + \not\partial_y)) (i(\not\partial q_\varepsilon \otimes q_\varepsilon) \\ &\quad * \kappa_t^{-,d-2} + (q_\varepsilon \otimes q_\varepsilon) * (A \kappa_t^{+,d-1}))(x, y), \\ \rho_t^R(x, y) &:= \mathbb{1}_{B_R(0)}(x) \mathbb{1}_{B_R(0)}(y) \operatorname{tr}_{\mathbb{C}^r} (i(\not\partial_x + \not\partial_y) \\ &\quad \times (i \not\partial_1 \kappa_t^{-,d-2} + A(x) \kappa_t^{+,d-1}))(x, y), \\ \sigma_t(x, y) &:= -[A, \operatorname{tr}_{\mathbb{C}^r} (A \kappa_t^{-,d} + i \not\partial_1 \kappa_t^{+,d-1})](x, y). \end{aligned}$$

We collect first some properties of the introduced integral kernels.

Corollary 5.2. Let $l, m, n \in \mathbb{N}_0$ with $m \geq n$. Let $t > 0, k \in \mathbb{N}$; then,

$$\kappa_t^{\pm,k} \in C_{m,n}^l(\mathbb{R}^{2d}),$$

and there are continuous functions h_k , such that

$$\|\kappa_t^{-,k}\|_{C_{m,n}^{l,S^1}(\mathbb{R}^{2d})} + \|\kappa_t^{+,k}\|_{C_{m,n}^{l,S^1}(\mathbb{R}^{2d})} \leq h_k(t) t^{k-\frac{l+d}{2}}.$$

Moreover, for $\varepsilon, R > 0$, and $\psi \in C_c^\infty(\mathbb{R}^d)$ with $\text{supp } \psi \subseteq B_R(0)$, we have

$$\rho_t^{\varepsilon, R}, \rho_t^R, \sigma_t \in C_{0,0}^{0,S^1}(\mathbb{R}^{2d}),$$

such that for some continuous functions h^1, h^2 ,

$$\|(\psi \otimes \psi) \rho_t^{\varepsilon, R}\|_{C_{0,0}^{0,S^1}(\mathbb{R}^{2d})} \leq h^1(t) t^{-\frac{1}{2}}, \quad \|\sigma_t\|_{C_{0,0}^{0,S^1}(\mathbb{R}^{2d})} \leq h^2(t).$$

Proof. We have for k odd, and $0 < t \leq t_0$,

$$\begin{aligned} \|\kappa_t^{-,k}\|_{C_{m,n}^{l,S^1}(\mathbb{R}^{2d})} &\leq \sum_{j=\frac{k-1}{2}}^{\infty} \|r_t^{2j+1}\|_{C_{m,n}^{l,S^1}(\mathbb{R}^{2d})} \\ &\leq \left(\sum_{j=k}^{\infty} \frac{C^j}{\prod_{i=1}^j \max(1, i - \frac{l+d}{2})} t^{j-k} \right) t^{k-\frac{l+d}{2}} \\ &=: h_k(t) t^{k-\frac{l+d}{2}}. \end{aligned}$$

For $k \geq 1$ even, and $0 < t \leq t_0$, we have

$$\begin{aligned} \|\kappa_t^{+,k}\|_{C_{m,n}^{l,S^1}(\mathbb{R}^{2d})} &\leq \sum_{j=\frac{k}{2}}^{\infty} \|r_t^{2j}\|_{C_{m,n}^{l,S^1}(\mathbb{R}^{2d})} \\ &\leq \left(\sum_{j=k}^{\infty} \frac{C^j}{\prod_{i=1}^j \max(1, i - \frac{l+d}{2})} t^{j-k} \right) t^{k-\frac{l+d}{2}} \\ &=: h_k(t) t^{k-\frac{l+d}{2}}. \end{aligned}$$

As a first consequence, we obtain the claimed estimate for σ_t since $d \geq 3$. Letting the involved derivatives fall on q_ε , which is a Schwartz function, we also verify the claimed estimate for $(\psi \otimes \psi) \rho_t^{\varepsilon, R}$. ■

If we apply Lemma 2.19 to Proposition 2.29 and Lemma 4.9, we obtain the following corollary.

Corollary 5.3. Denote for $R > 0$ $\chi_R := \mathbb{1}_{B_R(0)}$ the characteristic function of the ball of radius R . Then, for $t > 0$,

$$\begin{aligned} &\text{tr}_{\mathbb{C}^r}(e^{-tD^*D} - e^{-tDD^*}) \\ &= \lim_{R \rightarrow \infty} \int_0^t (\chi_R \text{tr}_{\mathbb{C}^r} ([i\partial, (i\partial K_s^{-,d-2} + AK_s^{+,d-1})]) \chi_R \\ &\quad - \chi_R [A, \text{tr}_{\mathbb{C}^r} (AK_s^{-,d} + i\partial K_s^{+,d-1})] \chi_R) ds, \end{aligned}$$

where the double limit is in $S^1(L^2(\mathbb{R}^d, H))$.

The next lemma is a table of all relevant integral kernels and the corresponding operators. Denote by P_ε the operator defined by

$$P_\varepsilon f := q_\varepsilon * f.$$

Lemma 5.4. *Let $t > 0$, $j \in \mathbb{N}_0$, $k \in \mathbb{N}$; then, for $f \in L^2(\mathbb{C}^r \otimes H)$, and a.e. $x \in \mathbb{R}^d$,*

$$\begin{aligned} \int_{\mathbb{R}^d} \theta_t^j(x, y) f(y) dy &= \left(\int_{s \in \Delta_j} e^{-sH_0} \sqcup (A^2 - M_0^2)^{\otimes j} ds f \right)(x), \\ \int_{\mathbb{R}^d} \theta_t(x, y) f(y) dy &= (e^{-tH_B} f)(x), \\ \int_{\mathbb{R}^d} r_t^j(x, y) f(y) dy &= (R_t^j f)(x), \\ \int_{\mathbb{R}^d} \kappa_t^{\pm, k}(x, y) f(y) dy &= (K_t^{\pm, k} f)(x), \end{aligned} \quad (59)$$

and for $t, \varepsilon, r > 0$, $f \in L^2(\mathbb{R}^d, H)$, and a.e. $x \in \mathbb{R}^d$,

$$\begin{aligned} \int_{\mathbb{R}^d} \rho_t^{\varepsilon, R}(x, y) f(y) dy \\ &= \overline{(\chi_R \text{tr}_{\mathbb{C}^r} ([i\partial, (i\partial P_\varepsilon K_t^{-, d-2} + P_\varepsilon A K_t^{+, d-1}) P_\varepsilon]) \chi_R f)}(x), \\ \int_{\mathbb{R}^d} \chi_R(x) \sigma_t(x, y) \chi_R(y) f(y) dy \\ &= -(\chi_R [A, \text{tr}_{\mathbb{C}^r} (A K_s^{-, d} + i\partial K_s^{+, d-1})] \chi_R f)(x). \end{aligned} \quad (60)$$

Proof. The pointwise estimates of the involved kernels by multiples of $q_t(x - y)$ enable us to use Fubini's theorem on appearing infinite sums and integrals and obtain successively the claimed integral kernel properties (59). For σ_t in (60), the claim follows also by Fubini's theorem, the memberships $\kappa_t^{\pm, k} \in C_{m, n}^{1, S^1}(\mathbb{R}^{2d})$, and the fact that χ_R is compactly supported. Furthermore,

$$\eta_t := (i\partial q_\varepsilon \otimes q_\varepsilon) * \kappa_t^{-, d-2} + (q_\varepsilon \otimes q_\varepsilon) * (A \kappa_t^{+, d-1})$$

is smooth, because q_ε is a Schwartz function. We also have for $f \in C_c^\infty(\mathbb{R}^d, \mathbb{C}^r)$, via integration by parts,

$$\begin{aligned} \int_{\mathbb{R}^d} (i(\partial_1 + \partial_2) \eta_t)(x, y) f(y) dy \\ &= i\partial((i\partial P_\varepsilon K_t^{-, d-2} + P_\varepsilon A K_t^{+, d-1}) P_\varepsilon) f \\ &\quad - i \sum_{j=1}^d c^j ((i\partial P_\varepsilon K_t^{-, d-2} + P_\varepsilon A K_t^{+, d-1}) P_\varepsilon) \partial_j f. \end{aligned}$$

We apply $\mathrm{tr}_{\mathbb{C}^r}$, change c^j to the end, and have, for $f \in C_c^\infty(\mathbb{R}^d, H)$,

$$\begin{aligned} & \int_{\mathbb{R}^d} \mathrm{tr}_{\mathbb{C}^r}((i(\not{\partial}_1 + \not{\partial}_2)\eta_t)(x, y))f(y)dy \\ &= \mathrm{tr}_{\mathbb{C}^r}([i\not{\partial}, (i\not{\partial}P_\varepsilon K_t^{-,d-2} + P_\varepsilon A K_t^{+,d-1})P_\varepsilon]f)(x). \end{aligned}$$

Since the right-hand side, due to the presence of P_ε , possesses a bounded extension (which must equal its closure) in $L^2(\mathbb{R}^d, H)$, we obtain the claim for $\rho_t^{\varepsilon,R}$ in (60). ■

Lemma 5.5. *Let $t > 0$. Then,*

$$\mathrm{tr}_{L^2(\mathbb{R}^d, H)} \mathrm{tr}_{\mathbb{C}^r} (e^{-tD^*D} - e^{-tDD^*}) = \mathrm{tr}_{\mathbb{C}^r \otimes H} \left(\lim_{R \rightarrow \infty} \int_{\mathbb{R}^d} \int_0^t \rho_s^R(x, x) ds dx \right).$$

The outer integral over $B_R(0)$ on the right is a Bochner integral in $L^1(\mathbb{R}^d, S^1(\mathbb{C}^r \otimes H))$, and the limit exists in trace-class of $\mathbb{C}^r \otimes H$.

Proof. We first consider for $s > 0$ the operator

$$-[A, A K_s^{-,d} + i\not{\partial} K_s^{+,d-1}],$$

which by Lemma 5.4 has the operator valued integral kernel

$$\sigma_s(x, y) := -[A, A \kappa_s^{-,d} + i\not{\partial}_1 \kappa_s^{+,d-1}](x, y).$$

We note that, by Corollary 5.2, $\sigma_s \in C_{m,n}^{0,S^1}(\mathbb{R}^{2d})$ for all $m \geq n$, $m, n \in \mathbb{N}_0$, with

$$\|\sigma_s\|_{C_{m,n}^{0,S^1}(\mathbb{R}^{2d})} \leq h(s)s^{d-1-\frac{d+1}{2}} = h(s)s^{\frac{d-3}{2}}$$

for some continuous h at 0. In particular, $s \rightarrow \sigma_s$ is integrable at 0 in $C_{m,n}^{0,S^1}(\mathbb{R}^{2d})$ -norm. Thus,

$$-\int_0^t [A, A K_s^{-,d} + i\not{\partial} K_s^{+,d-1}] ds$$

has the operator-valued integral kernel

$$\Sigma_t(x, y) := \int_0^t \sigma_s(x, y) ds.$$

For $R > 0$, the operator $\chi_R \mathrm{tr}_{\mathbb{C}^r} (e^{-tD^*D} - e^{-tDD^*}) \chi_R$ is trace-class in $L^2(\mathbb{R}^d, H)$ and admits by Theorem 4.2 an operator valued integral kernel $k_{t,R}$, such that

$$h \mapsto (x \mapsto k_{t,R}(x, x + h))$$

is a bounded continuous map of $\mathbb{R}^d$ to $L^1(\mathbb{R}^d, S^1(H))$. Because the kernel

$$\chi_R \otimes \chi_R \cdot \mathrm{tr}_{\mathbb{C}^r} \Sigma_t$$

is of the same class, Corollary 5.3 implies that the integral kernel $\int_0^t \rho_s^R ds$ is also of this class. In particular, Theorem 4.2 provides

$$\begin{aligned} & \operatorname{tr}_{L^2(\mathbb{R}^d, H)} (\chi_R \operatorname{tr}_{\mathbb{C}^r} (e^{-tD^*D} - e^{-DD^*}) \chi_R) \\ &= \int_{\mathbb{R}^d} \chi_R(x) \operatorname{tr}_{\mathbb{C}^r \otimes H} \Sigma_t(x, x) dx \\ &+ \int_{\mathbb{R}^d} \operatorname{tr}_H \left(\int_0^t \rho_s^R(x, x) ds \right) dx. \end{aligned}$$

We claim that the first summand vanishes, which would finish the proof after taking the limit $R \rightarrow \infty$. Indeed, first, we have $\tau_s(x, y) := A\kappa_s^{-,d} + i\theta_1\kappa_s^{+,d-1} \in C_{m,n}^{0,S^1}(\mathbb{R}^{2d})$ for all $m, n \in \mathbb{N}_0$ by Corollary 5.2, which implies, because $A(x)\langle A_0 \rangle^{-1}$ is a bounded operator, that

$$\operatorname{tr}_{\mathbb{C}^r \otimes H} A(x) \tau_s(x, x) = \operatorname{tr}_{\mathbb{C}^r \otimes H} \langle A_0 \rangle \tau_s(x, x) A(x) \langle A_0 \rangle^{-1} = \operatorname{tr}_{\mathbb{C}^r \otimes H} \overline{\tau_s(x, x) A(x)},$$

which implies that $\operatorname{tr}_{\mathbb{C}^r \otimes H} \sigma_s(x, x) = \operatorname{tr}_{\mathbb{C}^r \otimes H} [A(x), \tau(x, x)] = 0$. Then, also,

$$\operatorname{tr}_{\mathbb{C}^r \otimes H} \Sigma_t(x, x) = \int_0^t \operatorname{tr}_{\mathbb{C}^r \otimes H} \sigma_s(x, x) ds = 0.$$

The claim follows from Corollary 5.3. ■

Before we proceed with the term involving ρ_s^R , we need a technical lemma concerned with the decay of the Gaussian heat kernel outside compact regions. This result is classical and the technique is usually called dyadic exhaustion.

Lemma 5.6. *Let $u_j > 0$, $j = 0, \dots, k$ with $t_0 = \sum_{j=0}^k u_j$ and $r_0 > 0$. Let $\delta, \varepsilon \geq 0$. Then, for $c > 1$, there exists a constant C such that for $i, j = 1, \dots, k$, $x \in \mathbb{R}^d$*

$$\begin{aligned} & \int_{(\mathbb{R}^d)^k} \chi_{|z_i - x| \geq r_0} |x - z_1|^\delta |z_j - x|^\varepsilon q_{u_0}(x - z_1) q_{u_1}(z_1 - z_2) \cdots q_{u_k}(z_k - x) dz \\ & \leq C t_0 u_0^{\frac{\delta}{2}} U_j^{\frac{\varepsilon}{2}} r_0^{-d} \exp\left(-\frac{r_0^2}{2ct_0}\right), \end{aligned} \quad (61)$$

where

$$U_j := \begin{cases} u_0 + \cdots + u_{j-1}, & j < i, \\ u_j + \cdots + u_k, & j \geq i. \end{cases}$$

Proof. For $c > 1$ $\eta \geq 0$, there exists a constant $C_{c,\eta}$ such that

$$|y|^\eta q_s(y) \leq C_{c,\eta} s^{\frac{\eta}{2}} q_{cs}(y)$$

uniformly in $s > 0$ and $y \in \mathbb{R}^d$. This implies that (61) can be estimated by

$$C u_0^{\frac{\delta}{2}} U_j^{\frac{\varepsilon}{2}} \int_{\mathbb{R}^d} \chi_{|y| \geq r_0} q_{c(u_0 + \cdots + u_{i-1})}(y) q_{c(u_i + \cdots + u_k)}(y) dy$$

for $c > 1$ and some constant C . Let $r_n := 2^n r_0$ and $X_n := B_{r_n}(0) \setminus B_{r_{n-1}}(0)$. Then, $\text{vol } X_n \leq c d r_n^d$ and $q_s(y) \leq q_s(r_{n-1})$ for $y \in X_n$. Thus, for $c' > c$,

$$\begin{aligned} & C u_0^{\frac{\delta}{2}} U_j^{\frac{\varepsilon}{2}} \int_{\mathbb{R}^d} \chi_{|y| \geq r_0} q_c(u_0 + \dots + u_{i-1})(y) q_c(u_i + \dots + u_k)(y) dy \\ & \leq C' u_0^{\frac{\delta}{2}} U_j^{\frac{\varepsilon}{2}} \sum_{n=1}^{\infty} r_n^d q_c(u_0 + \dots + u_{i-1})(r_{n-1}) q_c(u_i + \dots + u_k)(r_{n-1}) \\ & \leq C'' u_0^{\frac{\delta}{2}} U_j^{\frac{\varepsilon}{2}} r_0^{-d} \int_{r_0^2}^{\infty} \exp\left(-\frac{r}{2c't_0}\right) dr \\ & = C''' t_0 u_0^{\frac{\delta}{2}} U_j^{\frac{\varepsilon}{2}} r_0^{-d} \exp\left(-\frac{r_0^2}{2c't_0}\right). \quad \blacksquare \end{aligned}$$

Before we may proceed with discussing the integral kernels, we need the following lemma dealing with translations of products of operators. We first introduce some notation.

For an elementary tensor of operator functions $\mathbf{T} := T_1 \otimes \dots \otimes T_n$ and a vector $\mathbf{y} = (y_1, \dots, y_n)$, define

$$\begin{aligned} \text{pr } \mathbf{T} &:= T_1 \cdot \dots \cdot T_n, \\ \tau_{\mathbf{y}} \mathbf{T} &:= \tau_{y_1} T_1 \otimes \dots \otimes \tau_{y_n} T_n. \end{aligned}$$

We extend pr multi-linearly to general tensors of operator functions. We then have the following decomposition. The proof is elementary and is done by induction in n .

Lemma 5.7. *Let*

$$\mathbf{T} = T_1 \otimes \dots \otimes T_n$$

be an elementary tensor of operator functions. Then,

$$\begin{aligned} & \text{pr}(\tau_{-\frac{\mathbf{y}}{2}} - \tau_{\frac{\mathbf{y}}{2}})^2 \mathbf{T} \\ &= \sum_{j=1}^n \left(\prod_{i=1}^{j-1} \tau_{y_i} T_i \right) w_{y_j}^2 T_j \left(\prod_{i=j+1}^n \tau_{-y_i} T_i \right) \\ &+ 2 \sum_{1 \leq k < l \leq n} \left(\prod_{i=1}^{k-1} T_i \right) \tau_{\frac{y_k}{2}} \delta_{\frac{y_k}{2}} T_k \left(\prod_{j=k+1}^{l-1} \tau_{y_j} T_j \right) \tau_{-\frac{y_l}{2}} \delta_{\frac{y_l}{2}} T_l \left(\prod_{m=l+1}^n \tau_{-y_m} T_m \right). \end{aligned}$$

We have the following vanishing lemma for one of the terms making up $\rho_s^{\varepsilon, R}$.

Lemma 5.8. *Let $j \in \{1, \dots, d\}$. Then,*

$$\lim_{R \rightarrow \infty} R^{d-1} \lim_{\varepsilon \searrow 0} \int_0^t \int_{S_1(0)} \left\| (\partial_{j,1}(q_\varepsilon \otimes q_\varepsilon * \kappa_s^{-, d-2}))(Ry, Ry) \right\|_{S^1(H)} dS_1(y) ds = 0. \quad (62)$$

Proof. For $x_0 \in \mathbb{R}^d$, and $\gamma \in \{0, 1\}^k$, define

$$\begin{aligned} S_\gamma^{x_0} &:= (S_{\gamma_1}^{x_0}, \dots, S_{\gamma_k}^{x_0}), \\ S_0^{x_0} &:= A^2 - A^2(x_0), \\ S_1^{x_0} &:= i\not{B}. \end{aligned}$$

We use the iterative definition of the function κ_s^j to obtain, for $x_0, x, y \in \mathbb{R}^d$, $s > 0$,

$$\begin{aligned} \kappa_s^{-,d-2}(x, y) &= \sum_{j=\frac{d-3}{2}}^{\infty} r_s^{2j+1}(x, y) \\ &= - \sum_{j=\frac{d-3}{2}}^{\infty} \sum_{k=2j+1}^{\infty} (-1)^k \sum_{\gamma \in \{0,1\}^k, |\gamma|=2j+1} \int_{u \in s\Delta_k} (Q_u^{x_0} \lrcorner S_\gamma^{x_0})(x, y) du, \quad (63) \end{aligned}$$

where the expression on the right converges absolutely in $C_{m,n}^{1,S^1}(\mathbb{R}^{2d})$ for $m, n \in \mathbb{N}_0$. We investigate $((\partial_j q_\varepsilon \otimes q_\varepsilon) * \kappa_s^{-,d-2})(Ry, Ry)$ for $R > 0$, $y \in S_1(0)$, and $x_0 = Ry$ using the above series. Since $\|Q_u^{x_0}\| \leq q_u$, we have the estimate

$$\begin{aligned} &\left\| \int_{u \in s\Delta_k} \partial_{j,1}(q_\varepsilon \otimes q_\varepsilon * (Q_u^x \lrcorner S_\gamma))(x, x) du \right\|_{S^1(H)} \\ &\leq s^k \int_{u \in \Delta_k} \int_{(\mathbb{R}^d)^k} \frac{|z_1^j|}{2(su_0 + \varepsilon)} q_{su_0 + \varepsilon}(z_1) \\ &\quad \cdot q_{su_1}(z_1 - z_2) \cdots q_{su_k + \varepsilon}(z_k) \prod_{i=1}^k \|S_{\gamma_i}^x(x + z_i)\|_{S^1(H)} dz du. \quad (64) \end{aligned}$$

We restrict the integral in $z \in (\mathbb{R}^d)^k$ to $z \in B_{r_0}(0)^k$ with $r_0 = \log |x|$. Since

$$\|S_{\gamma_i}^x\|_{L^\infty(\mathbb{R}^d, S^1(H))} \leq c$$

is uniformly bounded, the $2^k - 1$ resulting remainders can be estimated by Lemma 5.6 for $\varepsilon \in (0, 1)$,

$$\begin{aligned} &C(2^k - 1)c^k(t + 2)^{k+1}s^{-\frac{1}{2}}(\log |x|)^{-d} \int_{u \in \Delta_k} u_0^{-\frac{1}{2}} du \exp\left(-\frac{(\log |x|)^2}{2c'(t + 2)}\right) \\ &\leq C'(2c(t + 2))^{k+1}s^{-\frac{1}{2}} \frac{1}{(k - 1)!} |x|^{-\frac{\log |x|}{2c'(t+2)}}, \end{aligned}$$

for which the sum over k and the integral in $s \in (0, t)$ decays faster than any $|x|^{-m}$, $m \in \mathbb{N}$, as $|x| \rightarrow \infty$. We return to (64) with the integrals restricted to $z \in B_{r_0}(0)^k$ with

$r_0 = \log |x|$. Condition (43) of Remark 3.6 and the decay of $\|\nabla B(x)\|_{S^1(H)} \sim |x|^{-1}$ as $|x| \rightarrow \infty$, due to $\tau^{0,0,\nabla,1,1}(B) < \infty$, allows us to estimate by

$$\begin{aligned} & C c'^k (|x| - \log |x|)^{-\frac{1}{2}(2j+k+1)} s^{k-\frac{1}{2}} q_{c(s+2\varepsilon)}(0) \int_{u \in \Delta_k} u_0^{-\frac{1}{2}} du \\ & \leq C' \frac{c'^k s^{k-\frac{d+1}{2}}}{(k-1)!} (|x| - \log |x|)^{-k}, \end{aligned}$$

which shows absolute summability of (64) with respect to the sums in (63) and integrability in s at 0, uniformly in $\varepsilon \in (0, 1)$. We also note that, for the limit $|x| \rightarrow \infty$, we may disregard all terms involving the summands with $j \geq \frac{d-1}{2}$ or $j = \frac{d-3}{2}$, $k \geq d$, and it suffices for the statement (62) to hold that

$$\begin{aligned} & \lim_{R \rightarrow \infty} R^{d-1} \lim_{\varepsilon \searrow 0} \int_0^t s^{d-2} \int_{S_1(0)} \\ & \times \left\| \int_{u \in \Delta_{d-2}} \partial_{j,1} (q_\varepsilon \otimes q_\varepsilon * (Q_{su}^{Ry} \sqcup_* i\!\not\!B^{\otimes(d-2)}))(Ry, Ry) du \right\|_{S^1(H)} \\ & dS_1(y) ds = 0 \end{aligned} \quad (65)$$

and

$$\begin{aligned} & \lim_{R \rightarrow \infty} R^{d-1} \lim_{\varepsilon \searrow 0} \int_0^t s^{d-1} \int_{S_1(0)} \\ & \times \left\| \int_{u \in \Delta_{d-1}} \partial_{j,1} (q_\varepsilon \otimes q_\varepsilon * (Q_{su}^{Ry} \sqcup_* S_\gamma))(Ry, Ry) du \right\|_{S^1(H)} dS_1(y) ds = 0 \end{aligned} \quad (66)$$

for $\gamma \in \{0, 1\}^{d-1}$, $|\gamma| = d - 2$. We consider first the term in (65):

$$\begin{aligned} & \partial_{j,1} (q_\varepsilon \otimes q_\varepsilon * (Q_{su}^{Ry} \sqcup_* i\!\not\!B^{\otimes(d-2)}))(Ry, Ry) \\ & = - \int_{(\mathbb{R}^d)^{d-2}} \frac{Ry^j - w_1^j}{2(su_0 + \varepsilon)} q_{su_0 + \varepsilon}(Ry - w_1) q_{su_1}(w_1 - w_2) \\ & \quad \cdot \dots \cdot q_{su_{d-2} + \varepsilon}(w_{d-2} - Ry) e^{-su_0 A(Ry)^2} \prod_{j=1}^{d-2} i\!\not\!B(w_j) e^{-su_j A(Ry)^2} dw \\ & \stackrel{w \mapsto Ry + z}{=} - \int_{(\mathbb{R}^d)^{d-2}} \frac{z_1^j}{2(su_0 + \varepsilon)} q_{su_0 + \varepsilon}(z_1) q_{su_1}(z_1 - z_2) \cdot \dots \cdot q_{su_{d-2} + \varepsilon}(z_{d-2}) \\ & \quad \cdot e^{-su_0 A(Ry)^2} \prod_{j=1}^{d-2} i\!\not\!B(Ry + z_j) e^{-su_j A(Ry)^2} dz \end{aligned}$$

$$\begin{aligned} \stackrel{z \mapsto -z}{=} & - \int_{(\mathbb{R}^d)^{d-2}} \frac{z_1^j}{2(su_0 + \varepsilon)} q_{su_0 + \varepsilon}(z_1) q_{su_1}(z_1 - z_2) \cdots q_{su_{d-2} + \varepsilon}(z_{d-2}) \\ & \cdot e^{-su_0 A(Ry)^2} \prod_{j=1}^{d-2} i \not{B}(Ry - z_j) e^{-su_j A(Ry)^2} dz. \end{aligned}$$

Taking the sum, we obtain

$$\begin{aligned} & R^{d-1} \partial_{j,1} (q_\varepsilon \otimes q_\varepsilon * (Q_{su}^{Ry} \lrcorner_* i \not{B}^{\otimes(d-2)} - Q_{su}^{Ry} \lrcorner_* (i \not{B}(Ry))^{\otimes(d-2)}))(Ry, Ry) \\ & = -R^{d-1} \int_{(\mathbb{R}^d)^{d-2}} \frac{z_1^j}{4(su_0 + \varepsilon)} q_{su_0 + \varepsilon}(z_1) q_{su_1}(z_1 - z_2) \\ & \quad \cdot \cdots \cdot q_{su_{d-2} + \varepsilon}(z_{d-2}) e^{-su_0 A(Ry)^2} \\ & \quad \cdot [\text{pr}(\tau_{-\frac{z}{2}} - \tau_{\frac{z}{2}})^2 (i \not{B} e^{-su_1 A(Ry)^2}, \dots, i \not{B} e^{-su_{d-2} A(Ry)^2})](Ry) dz. \end{aligned} \quad (67)$$

We first note that, for all $\varepsilon > 0$,

$$\begin{aligned} & \partial_{j,1} (Q_{su}^{Ry} \lrcorner_* (i \not{B}(Ry))^{\otimes(d-2)})(Ry, Ry) \\ & = (\partial_{j,1} q_s)(Ry, Ry) \cdot [e^{-su A(Ry)^2} \lrcorner (i \not{B}(Ry))^{\otimes(d-2)}] = 0, \end{aligned}$$

which means we are left with discussing the term (67). As before, we can use Lemma 5.6 to restrict the integrals on the right-hand side of (67) to $z \in B_{\log R}(0)^{d-2}$ uniformly in $\varepsilon \in (0, 1)$. By Lemma 5.7, we see that $\text{pr}(\tau_{-\frac{z}{2}} - \tau_{\frac{z}{2}})^2$ decomposes into a finite sum of products that involve one factor $w_\bullet^2$ or two factors $\delta_\bullet$ applied to $i \not{B}$. One of these factors can be bounded on $z \in B_{\log R}(0)^{d-2}$ by the fact that $i \not{B}$ is continuously differentiable, and thus locally Lipschitz, while all other factors are estimated uniformly. In total, we may crudely estimate on $z \in B_{\log R}(0)^{d-2}$,

$$\begin{aligned} & \| [\text{pr}(\tau_{-\frac{z}{2}} - \tau_{\frac{z}{2}})^2 (i \not{B} e^{-su_1 A(Ry)^2}, \dots, i \not{B} e^{-su_{d-2} A(Ry)^2})](Ry) \|_{S^1(H)} \\ & \leq C_R (|z_1| + \cdots + |z_{d-2}|), \end{aligned}$$

where C_R depends on R . The restricted integrals to $z \in B_{\log R}(0)^{d-2}$ on the right-hand side of (67) can, therefore, be estimated by

$$C'_R \sum_{l=1}^{d-2} \int_{(\mathbb{R}^d)^{d-2}} \frac{|z_1| |z_l|}{4(su_0 + \varepsilon)} q_{su_0 + \varepsilon}(z_1) q_{su_1}(z_1 - z_2) \cdots q_{su_{d-2} + \varepsilon}(z_{d-2}) dz. \quad (68)$$

Since $|w|q_t(w) \leq Ct^{\frac{1}{2}}q_{ct}(w)$ for $c > 1$ and a constant C dependent only on c , we further estimate (68) by

$$\begin{aligned} & C'_R C (su_0 + \varepsilon)^{-\frac{1}{2}} (s + \varepsilon)^{\frac{1}{2}} q_{c(s+2\varepsilon)}(0) \\ & \leq C_{R,c} u_0^{-\frac{1}{2}} s^{-\frac{1}{2}} (s + 2\varepsilon)^{\frac{1-d}{2}} \leq C_{R,c} u_0^{-\frac{1}{2}} s^{-\frac{d}{2}}, \end{aligned}$$

which is integrable in $s \in (0, t)$ against s^{d-2} because $d \geq 3$, and integrable in $u \in \Delta_{d-2}$. By the dominated convergence theorem, we conclude that the left-hand side of (65) equals

$$\begin{aligned} & - \lim_{R \rightarrow \infty} R^{d-1} \int_0^t s^{d-2} \int_{S_1(0)} \int_{u \in \Delta_{d-2}} \int_{B_{\log R}(0)^{d-2}} \\ & \times \frac{z_1^j}{4su_0} q_{su_0}(z_1) q_{su_1}(z_1 - z_2) \cdots q_{su_{d-2}}(z_{d-2}) \\ & \| e^{-su_0 A(Ry)^2} [\text{pr}(\tau_{-\frac{z}{2}} - \tau_{\frac{z}{2}})^2 (\mathfrak{i} \not B e^{-su_1 A(Ry)^2}, \dots, \mathfrak{i} \not B e^{-su_{d-2} A(Ry)^2})] (Ry) \|_{S^1(H)} \\ & dz du dS_1(y) ds. \end{aligned} \quad (69)$$

As before, $\text{pr}(\tau_{-\frac{z}{2}} - \tau_{\frac{z}{2}})^2$ decomposes into a finite sum of products that involve one factor $w_\bullet^2$ or two factors $\delta_\bullet$ applied to $\mathfrak{i} \not B$. In any case, both can be bounded by condition (44), respectively, (45), of Remark 3.6 in such a way that their decay as $R \rightarrow \infty$ compensates the factor R^{d-1} , uniformly in s, y, u , and z . Here, the additional Hölder-type continuity at infinity in the case $d = 3$ from condition (44), respectively, (45) of Remark 3.6 goes in, to obtain the necessary integrability in s at 0. We are allowed to use the dominated convergence theorem and the summands involving factors $w_\bullet^2$ go to 0 as $R \rightarrow \infty$, by condition (47), while those with two $\delta_\bullet$ go to 0 as $R \rightarrow \infty$ by condition (44) for the same reason. We conclude that (69) vanishes.

The second type (66) is simpler. Let S_γ have $A^2 - A(Ry)^2$ in the j -th slot. Since

$$s^{d-1} \left\| \int_{u \in \Delta_{d-1}} Q_{su}^{Ry} \sqcup_* S_\gamma du \right\|_{C_{0,0}^{1,S^1}(\mathbb{R}^{2d})} \leq c s^{\frac{d-3}{2}},$$

for s near 0, uniformly in R and y , we see that we may pass the limit $\varepsilon \searrow 0$ by the integrals. Let $\tilde{S}_\gamma$ be obtained from S_γ by replacing all $\mathfrak{i} \not B$ by $\mathfrak{i} \not B(Ry)$. By an argument similar to the first type, we see that

$$\begin{aligned} & \lim_{R \rightarrow \infty} R^{d-1} \int_0^t s^{d-1} \int_{u \in \Delta_{d-1}} \left\| \partial_{j,1} (Q_{su}^{Ry} \sqcup_* S_\gamma \right. \\ & \left. - Q_{su}^{Ry} \sqcup_* \tilde{S}_\gamma)(Ry, Ry) \right\|_{S^1(H)} du ds = 0. \end{aligned}$$

But for the expression with $\tilde{S}_\gamma$, we have

$$\begin{aligned} & \partial_{j,1} (Q_{su}^{Ry} \sqcup_* \tilde{S}_\gamma)(Ry, Ry) \\ & = \int_{\mathbb{R}^d} (\partial_{j,1} q_{s(u_0 + \dots + u_{j-1})})(Ry - w_j) q_{s(u_j + \dots + u_{d-1})}(w_j - Ry) \\ & \times [e^{-suA(Ry)^2} \sqcup T_j(w_j)] dw_j, \end{aligned}$$

where T_j is the $(d-1)$ -vector of operator valued function which consists of $d-2$ constant operators $\mathfrak{i} \not B(Ry)$ and $A^2 - A^2(Ry)$ in the j -th slot. We now repeat the

trick of first changing coordinates $w_j \mapsto Ry + z_j$ and then $z_j \mapsto -z_j$ as before to obtain a factor $w_{z_j}^2(A^2)(Ry)$ in the j -th slot of the $\sqcup$ -product in the above equation. We then apply dominated convergence and condition (46) of Remark 3.6 to conclude that the second type also vanishes. ■

As an intermediate step to the trace formula, we show the following proposition. Denote, for $v \in \mathbb{R}^d$,

$$\langle c, v \rangle := \sum_{j=1}^d c^j v_j.$$

Proposition 5.9. *Let $t > 0$. Then,*

$$\begin{aligned} & \mathrm{tr}_{L^2(\mathbb{R}^d, H)} \mathrm{tr}_{\mathbb{C}^r} (e^{-tD^*D} - e^{-tDD^*}) \\ &= \mathrm{tr}_H \left(\lim_{R \rightarrow \infty} R^{d-1} \int_0^t \int_{S_1(0)} \mathrm{tr}_{\mathbb{C}^r} (i\langle c, y \rangle A(Ry) \kappa_s^{+, d-1}(Ry, Ry)) dS_1(y) ds \right), \end{aligned}$$

where the argument of tr_H on the right-hand side is a limit in $S^1(H)$ -norm.

Proof. In the proof of Lemma 5.5, we showed that there is an operator valued integral kernel η_t of the operator

$$\int_0^t \mathrm{tr}_{\mathbb{C}^r} ([i\partial, (i\partial K_s^{-, d-2} + A K_s^{+, d-1})]) ds,$$

such that with $\eta_t^R := (\chi_R \otimes \chi_R) \cdot \eta_t$ for all $R > 0$ the map

$$h \mapsto (x \mapsto \eta_t^R(x, x+h))$$

is a bounded continuous map of $\mathbb{R}^d$ to $L^1(\mathbb{R}^d, S^1(H))$. It follows that for $\delta > 0$ also

$$\sup_{h \in B_\delta(0)} \int_{B_R(0)} \|((q_\varepsilon \otimes q_\varepsilon) * \eta_t)(x, x+h) - \eta_t(x, x+h)\|_{S^1(H)} dx \xrightarrow{\varepsilon \searrow 0} 0.$$

Theorem 4.2 implies that

$$\begin{aligned} & \mathrm{tr}_{L^2(\mathbb{R}^d, H)} \int_0^t \chi_R \mathrm{tr}_{\mathbb{C}^r} ([i\partial, (i\partial K_s^{-, d-2} + A K_s^{+, d-1})]) \chi_R ds \\ &= \lim_{\varepsilon \searrow 0} \int_{B_R(0)} \mathrm{tr}_H ((q_\varepsilon \otimes q_\varepsilon) * \eta_t)(x, x) dx. \end{aligned}$$

On the other hand for $\varepsilon > 0$, we have by Corollary 5.2 that for $\psi \in C_c^\infty(\mathbb{R}^d)$ with $\mathrm{supp} \psi \subseteq B_R(0)$

$$\|\rho_s^{\varepsilon, R}\|_{C_{0,0}^{0, S^1}(\mathbb{R}^{2d})} \leq h(s) s^{-\frac{1}{2}}$$

for some continuous function h at 0. In particular, $\int_0^t \rho_s^{\varepsilon, R} ds$ exists in $C_{0,0}^{0,S^1}(\mathbb{R}^{2d})$ and thus needs to coincide with $(q_\varepsilon \otimes q_\varepsilon) * \eta_t$ on $B_R(0) \times B_R(0)$. This implies that we may interchange the trace and integrals freely to obtain

$$\int_{B_R(0)} \mathrm{tr}_H((q_\varepsilon \otimes q_\varepsilon) * \eta_t)(x, x) dx = \int_0^t \mathrm{tr}_H \int_{B_R(0)} \rho_s^{\varepsilon, R}(x, x) dx ds. \quad (70)$$

We consider the innermost integral of the right-hand side of (70) in the weak operator topology of H . Then, the divergence theorem applies, and we have after changing to polar coordinates,

$$\begin{aligned} & \int_{B_R(0)} \rho_s^{\varepsilon, R}(x, x) dx \\ &= R^{d-1} \int_{S_1(0)} \mathrm{tr}_{\mathbb{C}^r}(\mathrm{i}\langle c, y \rangle (\mathrm{i} \not{D} q_\varepsilon \otimes q_\varepsilon) * \kappa_s^{-, d-2}(Ry, Ry)) dS_1(y) \\ &+ R^{d-1} \int_{S_1(0)} \mathrm{tr}_{\mathbb{C}^r}(\mathrm{i}\langle c, y \rangle (q_\varepsilon \otimes q_\varepsilon) * (A\kappa_s^{+, d-1})(Ry, Ry)) dS_1(y). \end{aligned} \quad (71)$$

We note that in the second summand on the right-hand side of (71) the kernel $A\kappa_s^{+, d-1}$ is of class $C_{0,0}^{1,S^1}(\mathbb{R}^{2d})$ with norm bounded by $h(s)s^{\frac{d-3}{2}}$ for some continuous h by Corollary 5.2, which is integrable in s at 0. In particular, after applying the divergence theorem in reverse on the second summand of (71), we may take the limit $\varepsilon \searrow 0$ inside the trace, and thus,

$$\begin{aligned} & \lim_{\varepsilon \searrow 0} \mathrm{tr}_H \left(R^{d-1} \int_{S_1(0)} \mathrm{tr}_{\mathbb{C}^r}(\mathrm{i}\langle c, y \rangle (q_\varepsilon \otimes q_\varepsilon) * (A\kappa_s^{+, d-1})(Ry, Ry)) dS_1(y) \right) \\ &= \mathrm{tr}_H \left(R^{d-1} \int_{S_1(0)} \mathrm{tr}_{\mathbb{C}^r}(\mathrm{i}\langle c, y \rangle A(Ry) \kappa_s^{+, d-1}(Ry, Ry)) dS_1(y) \right). \end{aligned}$$

We are left with the first summand on the right-hand side of (71). Its contribution vanishes in the iterative limit $\lim_{R \rightarrow \infty} \lim_{\varepsilon \searrow 0}$, by Lemma 5.8. The claim then follows from Lemma 5.5. $\blacksquare$

6. The principal trace formula

In this section, we exploit that we only need the involved integral kernels in their long-range limits $|x| \rightarrow \infty$. The first result shows that we do not need to care about which values the operator family A has near 0.

Lemma 6.1. *For $j \in \mathbb{N}$, let $M = (M_i)_{i=1}^j$ be measurable families of bounded operators in $\mathbb{C}^{r \times r} \otimes \langle A_0 \rangle^{-n} B(H) \langle A_0 \rangle^{-m}$, with*

$$\|M_i(x)\|_{L^\infty(\mathbb{R}^d, \mathbb{C}^{r \times r} \otimes \langle A_0 \rangle^{-n} B(H) \langle A_0 \rangle^{-m})} \leq C,$$

for some constant $C < \infty$. Assume also that there are measurable functions

$$(0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d \ni (t, x, y) \mapsto k_t^i(x, y) \in \mathbb{C}^{r \times r} \otimes B(H), \quad i \in \{0, \dots, j\},$$

satisfying for some constant $c < \infty$,

$$\|k_t^i(x, y)\|_{B(\mathbb{C}^r \otimes \text{Dom } A_0^n)} \leq e^{ct} q_t(x - y), \quad x, y \in \mathbb{R}^d, \quad t > 0.$$

Denote for $R > 0$, $M' := (M'_i)_{i=1}^j$, with $M'_i \in \{M_i, M_i \mathbb{1}_{B_{\frac{R}{2}}(0)^c}\}$, $i \in \{1, \dots, j\}$, with at least one $i_0 \in \{1, \dots, j\}$, such that

$$M'_{i_0} = M_{i_0} \mathbb{1}_{B_{\frac{R}{2}}(0)^c}.$$

Then, there is a constant c' independent of j , such that, for $t > 0$,

$$\begin{aligned} & \int_{S_R(0)} \int_{s \in t \Delta_j} \|(k_s \wr_* M - k_s \wr_* M')(x, x)\|_{\mathbb{C}^{r \times r} \otimes \langle A_0 \rangle^{-n} B(H) \langle A_0 \rangle^{-m}} ds \, dS_R(x) \\ & \leq c' e^{ct} \frac{(2Ct)^j}{j!} R^{-1}. \end{aligned}$$

Proof. Since M and M' are uniformly bounded in $\|\cdot\|_{\mathbb{C}^{r \times r} \otimes \langle A_0 \rangle^{-n} B(H) \langle A_0 \rangle^{-m}}$ -norm by some constant C , we have, for $t > 0$, $x \in S_R(0)$,

$$\begin{aligned} & \int_{s \in t \Delta_j} \|(k_s \wr_* M - k_s \wr_* M')(x, x)\|_{\mathbb{C}^{r \times r} \otimes \langle A_0 \rangle^{-n} B(H) \langle A_0 \rangle^{-m}} ds \\ & \leq e^{ct} C^j (2^j - 1) \int_0^t \frac{u^{j-1}}{(j-1)!} \int_{B_{\frac{R}{2}}(0)} q_{t-u}(x-y) q_u(y-x) dy \, du. \end{aligned} \quad (72)$$

Since $\text{dist}(x, y) \geq \frac{R}{2}$, there exist constants c_d, c'_d only dependent on d , such that

$$\begin{aligned} & \int_{B_{\frac{R}{2}}(0)} q_{t-u}(x-y) q_u(y-x) du \\ & \leq R^d c_d \left(\sup_{\sigma > 0} \sigma^{-\frac{d}{2}} e^{-\frac{R^2}{16\sigma}} \right)^2 \stackrel{\lambda = \frac{R^2}{\sigma}}{=} R^d c_d \left(R^{-d} \sup_{\lambda > 0} \lambda^{\frac{d}{2}} e^{-\frac{\lambda}{16}} \right)^2 \\ & = c'_d R^{-d}. \end{aligned} \quad (73)$$

Compiling (72) and (73), we obtain

$$\begin{aligned} & \int_{s \in t \Delta_j} \|(k_s \wr_* M - k_s \wr_* (M \mathbb{1}_{B_{\frac{R}{2}}(0)^c}))(x, x)\|_{\mathbb{C}^{r \times r} \otimes \langle A_0 \rangle^{-n} B(H) \langle A_0 \rangle^{-m}} ds \\ & \leq e^{ct} c'_d C^j (2^j - 1) \frac{t^j}{j!} R^{-d}. \end{aligned}$$

Integration over $S_R(0)$ yields the claim. ■

Lemma 6.2. *Let $j \geq d$, and let $F := (F_k)_{k=1}^j$ be a tuple of measurable $B(\mathbb{C}^r \otimes H)$ -valued functions, which satisfy*

$$\|\langle X \rangle F_k\|_{L^\infty(\mathbb{R}^d, \mathbb{C}^{r \times r} \otimes \langle A_0 \rangle^{-n} B(H) \langle A_0 \rangle^{-m})} \leq C < \infty.$$

Let there be measurable functions

$$(0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d \ni (t, x, y) \mapsto k_t^i(x, y) \in B(\mathbb{C}^r \otimes \text{Dom } A_0^n), \quad i \in \{0, \dots, j\},$$

satisfying for some constant $c < \infty$,

$$\|k_t^i(x, y)\|_{B(\mathbb{C}^r \otimes \text{Dom } A_0^n)} \leq e^{ct} q_t(x - y), \quad x, y \in \mathbb{R}^d, \quad t > 0.$$

Then, for $t_0 > 0$, there is a constant C' independent of j , such that for $0 < t \leq t_0$, $R > 0$,

$$\begin{aligned} & \int_{S_R(0)} \int_{s \in t \Delta_j} \|(k_s \wr_* F)(x, x)\|_{\mathbb{C}^{r \times r} \otimes \langle A_0 \rangle^{-n} B(H) \langle A_0 \rangle^{-m}} ds \, dx \\ & \leq C' e^{ct} \frac{(2C)^j}{j!} t^{j - \frac{d}{2}} R^{-1}. \end{aligned}$$

Proof. Let $R > 0$ and consider first that all F_k are supported outside of $B_{\frac{R}{2}}(0)$. Then,

$$R \|F_k(x)\|_{\mathbb{C}^{r \times r} \otimes \langle A_0 \rangle^{-n} B(H) \langle A_0 \rangle^{-m}} \leq 2C,$$

for a.e. $x \in \mathbb{R}^d$. So,

$$\begin{aligned} & \int_{S_R(0)} \int_{s \in t \Delta_j} \|(k_s \wr_* F)(x, x)\|_{\mathbb{C}^{r \times r} \otimes \langle A_0 \rangle^{-n} B(H) \langle A_0 \rangle^{-m}} ds \, dx \\ & \leq e^{ct} (4\pi t)^{-\frac{d}{2}} \frac{(2Ct)^j}{j!} \text{vol } S_R(0) R^{-j} \\ & \leq C' e^{ct} \frac{(2C)^j}{j!} t^{j - \frac{d}{2}} R^{-1}. \end{aligned}$$

The general case follows by Lemma 6.1. ■

We are now ready to simplify the right-hand side of the principal trace formula to its penultimate form, which has its own *raison d'être*, in so far as it exhibits clearly a similar form as the classical Callias index formula (i.e., both exhibit a limit of a $d - 1$ form integrated over spheres with radii tending to infinity). However, it is not the final form, because we should not forget that

$$A = A_{n,m,l}$$

is still an approximant. Our general conditions on the family A do not suffice to enable us to go to the limit $n, m, l \rightarrow \infty$ in the trace formula of the lemma below.

Lemma 6.3. For $t > 0$,

$$\begin{aligned} & \operatorname{tr}_{L^2(\mathbb{R}^d, H)} \operatorname{tr}_{\mathbb{C}^r} (e^{-tD^*D} - e^{-tDD^*}) \\ &= \operatorname{tr}_H \left(\lim_{R \rightarrow \infty} R^{d-1} \int_0^t (4\pi s)^{-\frac{d}{2}} i^d \kappa_c \int_{S_1(0)} A(Ry) \int_{u \in s\Delta_{d-1}} \sum_{j=1}^d \sum_{\alpha \in \{1, \dots, d\}^{d-1}} \right. \\ & \quad \left. y^j \varepsilon_{(j, \alpha)} e^{-uA(Ry)^2} \sqcup ((\partial_{\alpha_1}^E A)(Ry), \dots, (\partial_{\alpha_{d-1}}^E A)(Ry)) du \, dS_1(y) \, ds \right), \end{aligned}$$

where $\varepsilon_{(j, \alpha)}$ denotes the Levi-Civita symbol of the tuple $(j, \alpha) \in \{1, \dots, d\}^d$.

Proof. For $x_0 \in \mathbb{R}^d$, denote

$$(M_{x_0} f)(x) := A(x_0) f(x), \quad x \in \mathbb{R}^d, \quad f \in \operatorname{Dom} M_0,$$

and

$$H_{x_0} := \Delta + M_{x_0}^2,$$

which is self-adjoint on $\operatorname{Dom} H_0$. The smooth integral kernel $Q_t^{x_0}$ of $e^{-tH_{x_0}}$, $t > 0$, is given by

$$Q_t^{x_0}(x, y) = q_t(x - y) \mathbb{1}_{\mathbb{C}^r} \otimes e^{-tA(x_0)^2}, \quad x, y \in \mathbb{R}^d.$$

Duhamel's principle yields

$$e^{-tH_B} = e^{-tH_{x_0}} - \int_0^t e^{-(t-s)H_{x_0}} (A^2 - M_{x_0}^2) e^{-sH_B} ds,$$

which implies for a.e. $x, y \in \mathbb{R}^d$,

$$\theta_t(x, y) = Q_t^{x_0}(x, y) - \int_0^t \int_{\mathbb{R}^d} Q_{t-s}^{x_0}(x, z) (A(z)^2 - A(x_0)^2) \theta_s(z, y) dz \, ds. \quad (74)$$

In fact, the right-hand side is an element of $C_{m,n}^\infty(\mathbb{R}^{2d})$, $m, n \in \mathbb{N}_0$, which can be shown by using Lemma 4.12, Corollaries 4.14 and 4.16 in a similar way as (57) and (58). So, (74) holds everywhere. We find

$$\begin{aligned} & r_t^{d-1}(x_0, x_0) \\ &= \int_{s \in t\Delta_{d-1}} ((Q_{s_0}^{x_0}, \theta_{s_1}, \dots, \theta_{s_{d-1}}) \sqcup_* (i\not{B})^{\otimes(d-1)})(x_0, x_0) ds \\ & \quad - \int_{s \in t\Delta_d} ((Q_{s_0}^{x_0}, \theta_{s_1}, \dots, \theta_{s_d}) \sqcup_* (A^2 - A(x_0)^2, (i\not{B})^{\otimes(d-1)}))(x_0, x_0) ds. \end{aligned}$$

By Lemma 6.1, we have for $n, m \in \mathbb{N}_0$, with $A(x)\langle A_0 \rangle^{-1} \leq C'$, $x \in \mathbb{R}^d$, and $B_{x_0} := A^2 - A(x_0)^2$,

$$\begin{aligned}
& \limsup_{R \rightarrow \infty} \int_0^t \int_{S_R(0)} \int_{u \in s \Delta_d} \|A(x_0)((\mathcal{Q}_{u_0}^{x_0}, \theta_{(u_1, \dots, u_d)}) \lrcorner_* (B_{x_0}, (\mathfrak{i} \not B)^{\otimes(d-1)})) \\
& \quad \times (x_0, x_0) \|_{\mathbb{C}^{r \times r} \otimes \langle A_0 \rangle^{-n} B(H) \langle A_0 \rangle^{-m}} du dS_R(x_0) ds \\
& = \limsup_{R \rightarrow \infty} \int_0^t \int_{S_R(0)} \int_{u \in s \Delta_d} \|A(x_0)((\mathcal{Q}_{u_0}^{x_0}, \theta_{(u_1, \dots, u_d)}) \\
& \quad \times \lrcorner_* (B_{x_0}, (\mathbb{1}_{B_{\frac{R}{2}}(0)} \mathfrak{i} \not B)^{\otimes(d-1)}))(x_0, x_0) \|_{\mathbb{C}^{r \times r} \otimes \langle A_0 \rangle^{-n} B(H) \langle A_0 \rangle^{-m}} \\
& \quad \times du dS_R(x_0) ds \\
& \leq C' C^{d-1} \limsup_{R \rightarrow \infty} \int_0^t e^{cs} \int_{S_1(0)} \int_0^s \int_{\mathbb{R}^d} q_{s-u}(Ry - z) \\
& \quad \times \|A(z)^2 - A(Ry)^2\|_{B(H, \text{Dom } A_0)} q_u(z - Ry) dz \frac{u^{d-1}}{(d-1)!} du dS_1(y) ds \\
& = C' C^{d-1} \limsup_{R \rightarrow \infty} \int_0^t e^{cs} \int_{S_1(0)} \int_0^s \int_{\mathbb{R}^d} q_{s-u}(w) q_u(w) \\
& \quad \times \|A(Ry + w)^2 - A(Ry)^2\|_{B(H, \text{Dom } A_0)} dw \frac{u^{d-1}}{(d-1)!} du dS_1(y) ds. \quad (75)
\end{aligned}$$

The integrand of the last line of (75) has an integrable dominant, since

$$\|A(Ry + w)^2 - A(Ry)^2\|_{B(H, \text{Dom } A_0)}$$

is uniformly bounded (since the function B is uniformly bounded with values in $\langle A_0 \rangle^{-m} B(H) \langle A_0 \rangle^n$ for any $m, n \in \mathbb{N}_0$), and we may take the limit $R \rightarrow \infty$ inside the integrals, which yields 0. Therefore,

$$\begin{aligned}
& \lim_{R \rightarrow \infty} R^{d-1} \int_0^t \int_{S_1(0)} \text{tr}_{\mathbb{C}^r} (\mathfrak{i} \langle c, y \rangle A(Ry) r_s^{d-1}(Ry, Ry)) dS_1(y) ds \\
& = \lim_{R \rightarrow \infty} R^{d-1} \int_0^t \int_{S_1(0)} \text{tr}_{\mathbb{C}^r} \left(\mathfrak{i} \langle c, y \rangle A(Ry) \right. \\
& \quad \times \left. \int_{u \in s \Delta_{d-1}} ((\mathcal{Q}_{u_0}^{Ry}, \theta_{u_1, \dots, u_{d-1}}) \lrcorner_* (\mathfrak{i} \not B)^{\otimes(d-1)})(Ry, Ry) du \right) dS_1(y) ds.
\end{aligned}$$

By iterating the procedure, we obtain

$$\begin{aligned}
& \lim_{R \rightarrow \infty} R^{d-1} \int_0^t \int_{S_1(0)} \text{tr}_{\mathbb{C}^r} (\mathfrak{i} \langle c, y \rangle A(Ry) r_s^{d-1}(Ry, Ry)) dS_1(y) ds \\
& = \lim_{R \rightarrow \infty} R^{d-1} \int_0^t \int_{S_1(0)} \text{tr}_{\mathbb{C}^r} (\mathfrak{i} \langle c, y \rangle A(Ry) p_s(Ry)) dS_1(y) ds,
\end{aligned}$$

where for $t > 0$, $x_0 \in \mathbb{R}^d$ we define

$$p_t(x_0) := \int_{s \in t \Delta_{d-1}} (Q_s^{x_0} \lrcorner_* (\mathfrak{i} \not{B})^{\otimes(d-1)})(x_0, x_0) ds.$$

Denote $(N_{x_0} f)(x) := (\mathfrak{i} \not{B})(x_0) f(x)$, $f \in \text{Dom } M_0$; then,

$$\begin{aligned} & \limsup_{R \rightarrow \infty} \int_0^t \int_{S_R(0)} \int_{u \in s \Delta_{d-1}} \|A(x_0) Q_u^{x_0} \lrcorner_* (\mathfrak{i} \not{B}) - N_{x_0}, (\mathfrak{i} \not{B})^{\otimes(d-2)}\| \\ & \quad \times (x_0, x_0) \|_{\mathbb{C}^{r \times r} \otimes B(H)} du dS_R(x_0) ds \\ &= \limsup_{R \rightarrow \infty} \int_0^t \int_{S_R(0)} \int_{u \in s \Delta_{d-1}} \|A(x_0) (Q_u^{x_0} \lrcorner_* (\mathfrak{i} \not{B}) \\ & \quad - N_{x_0}, (\mathbb{1}_{B_{\frac{R}{2}}(0)} \mathfrak{i} \not{B}))^{\otimes(d-2)})(x_0, x_0) \|_{\mathbb{C}^{r \times r} \otimes B(H)} du dS_R(x_0) ds \\ &\leq C' C^{d-1} \limsup_{R \rightarrow \infty} \int_0^t e^{cs} \int_{S_1(0)} \int_0^s \int_{\mathbb{R}^d} q_{s-u}(Ry - z) R \|(\not{B})(z) \\ & \quad - (\not{B})(Ry) \|_{B(H, \text{Dom } A_0)} q_u(z - Ry) dz \frac{u^{d-2}}{(d-2)!} du dS_1(y) ds \\ &= C' C^{d-1} \limsup_{R \rightarrow \infty} \int_0^t e^{cs} \int_{S_1(0)} \int_0^s \int_{\mathbb{R}^d} R \|(\not{B})(Ry + w) \\ & \quad - (\not{B})(Ry) \|_{B(H, \text{Dom } A_0)} q_{s-u}(w) q_u(w) dw \frac{u^{d-2}}{(d-2)!} du dS_1(y) ds. \quad (76) \end{aligned}$$

By the same reasoning as for (75), we may take the limit $R \rightarrow \infty$ inside the integrals in (76), which is 0. Thus,

$$\begin{aligned} & \lim_{R \rightarrow \infty} R^{d-1} \int_0^t \int_{S_1(0)} \text{tr}_{\mathbb{C}^r} (\mathfrak{i} \langle c, y \rangle A(Ry) p_s(Ry)) dS_1(y) ds \\ &= \lim_{R \rightarrow \infty} R^{d-1} \int_0^t \int_{S_1(0)} \text{tr}_{\mathbb{C}^r} \left(\mathfrak{i} \langle c, y \rangle A(Ry) \right. \\ & \quad \times \left. \int_{u \in s \Delta_{d-1}} (Q_u^{Ry} \lrcorner_* (N_{Ry}, (\mathfrak{i} \not{B})^{\otimes(d-2)}))(Ry, Ry) \right) dS_1(y) ds. \end{aligned}$$

By iterating the procedure, we obtain

$$\begin{aligned} & \lim_{R \rightarrow \infty} R^{d-1} \int_0^t \int_{S_1(0)} \text{tr}_{\mathbb{C}^r} (\mathfrak{i} \langle c, y \rangle A(Ry) p_s(Ry)) dS_1(y) ds \\ &= \lim_{R \rightarrow \infty} R^{d-1} \int_0^t \int_{S_1(0)} \text{tr}_{\mathbb{C}^r} (\mathfrak{i} \langle c, y \rangle A(Ry) \pi_s(Ry)) dS_1(y) ds, \end{aligned}$$

where for $t > 0$, $x_0 \in \mathbb{R}^d$,

$$\begin{aligned}\pi_t(x_0) &:= \int_{s \in t\Delta_{d-1}} (Q_s^{x_0} \sqcup_* (N_{x_0})^{\otimes(d-1)})(x_0, x_0) ds \\ &= (4\pi t)^{-\frac{d}{2}} \int_{s \in t\Delta_{d-1}} (\mathbb{1}_{\mathbb{C}^r}^{\otimes d} \otimes e^{-sA(x_0)^2}) \sqcup (\mathbf{i}(\not{B})(x_0))^{\otimes(d-1)} ds.\end{aligned}$$

The claim then follows if we apply $\mathrm{tr}_{\mathbb{C}^r}$ to $\mathbf{i}\langle c, y \rangle \pi_s$, using Lemma 2.1. $\blacksquare$

6.1. The main result

Throughout the previous sections, we used tacitly the approximation family $B_{n,m,l}$ instead of B for notational brevity. Now, we are prepared to take the limits $n \rightarrow \infty$, $m \rightarrow \infty$, $l \rightarrow \infty$ to arrive at the principal trace formula, which is our main result, presented in the following theorem.

If we assume Hypothesis 2.12, by Remark 2.13, the model operator A_0 is allowed to be $A(x_0)$, for a.e. $x_0 \in \mathbb{R}^d$. We fix such a x_0 and set $A_0 = A(x_0)$ in the following.

Theorem 6.4. *Assume Hypothesis 2.12. For $\phi \in C_c^\infty(\mathbb{R}^d)$, denote*

$$A_\phi := A_0 + (1 - \phi)(A - A_0).$$

Then, for $t > 0$, and any $\phi \in C_c^\infty(\mathbb{R}^d)$,

$$\begin{aligned}\mathrm{tr}_{L^2(\mathbb{R}^d, H)} \mathrm{tr}_{\mathbb{C}^r} (e^{-tD^*D} - e^{-tDD^*}) \\ = \frac{2}{d} (4\pi)^{-\frac{d}{2}} \mathbf{i}^d \kappa_c t^{\frac{d}{2}} \int_{s \in \Delta_{d-1}} \int_{\mathbb{R}^d} \mathrm{tr}_H \bigwedge_{j=0}^{d-1} ((dA_\phi) e^{-ts_j A_\phi^2}) ds,\end{aligned}\quad (77)$$

where $\bigwedge$ denotes the exterior product, and $\kappa_c = \mathrm{tr}_{\mathbb{C}^r}(c^1 \dots c^d)$. In case of the irreducible choice

$$r = 2^{\frac{d-1}{2}},$$

we have $\kappa_c = (2\mathbf{i})^{\frac{d-1}{2}} (-\mathbf{i})^d$ (see Lemma 2.1).

Proof. Denote $A_* := A_{n,m,l}$, and $D_* := D_{n,m,l}$. Let $r = |x|$. For $x = ry \in \mathbb{R}^d$ with $y \in S_1(0)$, we have $dr = \sum_{j=1}^d y^j dx^j$, and for $u \in s\Delta_{d-1}$, $s > 0$, we have

$$\begin{aligned}dr \wedge e^{-u_0 A_*^2} \bigwedge_{j=1}^{d-1} (dA_*) e^{-u_j A_*^2} \\ = \sum_{j=1}^d \sum_{\alpha \in \{1, \dots, d\}^{d-1}} y^j \varepsilon_{(j, \alpha)} e^{-u A_*^2} \sqcup (\partial_{\alpha_1}^E A_*, \dots, \partial_{\alpha_{d-1}}^E A_*) dx.\end{aligned}$$

If we apply $\iota_{dr^\#}$, the interior multiplication with the radial field, to both sides and restrict to $S_R(0)$, we obtain

$$\begin{aligned} & e^{-u_0 A_*^2} \bigwedge_{j=1}^{d-1} (dA_*) e^{-u_j A_*^2} \\ &= \sum_{j=1}^d \sum_{\alpha \in \{1, \dots, d\}^{d-1}} y^j \varepsilon_{(j, \alpha)} e^{-u A_*^2} \sqcup (\partial_{\alpha_1}^E A_*, \dots, \partial_{\alpha_{d-1}}^E A_*) dS_R(x). \end{aligned} \quad (78)$$

We insert (78) into Lemma 6.3 and change variables in the u -integration,

$$\begin{aligned} X_t &:= \operatorname{tr}_{L^2(\mathbb{R}^d, H)} \operatorname{tr}_{\mathbb{C}^r} (e^{-tD_*^* D_*} - e^{-tD_* D_*^*}) \\ &= i^d (4\pi)^{-\frac{d}{2}} \kappa_c \operatorname{tr}_H \left(\lim_{R \rightarrow \infty} \int_0^t s^{\frac{d}{2}-1} \int_{S_R(0)} A_* \int_{u \in \Delta_{d-1}} \right. \\ &\quad \left. \times e^{-su_0 A_*^2} \bigwedge_{j=1}^{d-1} (dA_*) e^{-su_j A_*^2} du ds \right). \end{aligned} \quad (79)$$

Due to the limit $R \rightarrow \infty$, we may replace A_* by $A_{\phi,*} := A_0 + (1 - \phi)(A_* - A_0)$, for any $\phi \in C_c^\infty(\mathbb{R}^d)$, in (79). We note that the integrand is Bochner integrable in trace-class, since dA_* is finite rank. We apply Stokes' theorem, and the trace tr_H , and get

$$X_t = i^d (4\pi)^{-\frac{d}{2}} \kappa_c \int_0^t s^{\frac{d}{2}-1} \int_{\mathbb{R}^d} (\omega_s^1 + \omega_s^2) ds, \quad (80)$$

where

$$\begin{aligned} \omega_s^1 &:= \int_{u \in \Delta_{d-1}} \operatorname{tr}_H \bigwedge_{j=0}^{d-1} ((dA_{\phi,*}) e^{-su_j A_{\phi,*}^2}) du, \\ \omega_s^2 &:= -2s \int_{u \in \Delta_d} \operatorname{tr}_H \left(A_{\phi,*}^2 e^{-su_0 A_{\phi,*}^2} \bigwedge_{j=1}^d (dA_{\phi,*}) e^{-su_j A_{\phi,*}^2} \right) du \\ &= -2s \int_{u \in \Delta_{d-1}} u_0 \operatorname{tr}_H \left((dA_{\phi,*}) e^{-su_0 A_{\phi,*}^2} A_{\phi,*}^2 \bigwedge_{j=1}^{d-1} (dA_{\phi,*}) e^{-su_j A_{\phi,*}^2} \right) du. \end{aligned}$$

By cyclically commuting the factor $A_{\phi,*}^2$ under the trace and changing variables, we obtain for ω_s^2 ,

$$\omega_s^2 = \frac{2}{d} s \partial_s \omega_s^1.$$

Integrating by parts in (80), we thus obtain

$$X_t = \frac{2}{d} (4\pi)^{-\frac{d}{2}} t^{\frac{d}{2}} i^d \kappa_c \int_{\mathbb{R}^d} \omega_t^1. \quad (81)$$

The argument of the trace of the n, m, l -dependent ω_l^1 possesses iteratively integrable dominants in trace-norm. Indeed, first, for fixed $n, m \in \mathbb{N}$, there exists a constant C independent of l (because K_m is finite rank), such that

$$\begin{aligned} & \left\| \bigwedge_{j=0}^{d-1} ((dA_{\phi,n,m,l})e^{-su_j A_{\phi,n,m,l}^2})(x) \right\|_{S^1(H)} \\ & \leq C \left\| \delta_l(K_m P_n B P_n K_m) \right\|_{\mathcal{F}_\varepsilon}^d \langle x \rangle^{-d-\varepsilon} dx \\ & \stackrel{\text{Lemma 3.2}}{\leq} C' \left\| K_m P_n B P_n K_m \right\|_{\mathcal{F}_\varepsilon}^d \langle x \rangle^{-d-\varepsilon} dx, \end{aligned}$$

which is an integrable dominant on $\mathbb{R}^d \times \Delta_{d-1}$, and thus allows us to take the limit $l \rightarrow \infty$ under the integral.

Now, fix n . Since

$$B(x_0) = A(x_0) - A_0 = 0,$$

the operator function $\langle A_0 \rangle^{-\alpha+\beta} B \langle A_0 \rangle^{-\beta}$ is Lipschitz with values in $S^d(H)$, for α, β as in Hypothesis 2.12. Since $\nabla \phi$ is compactly supported, it follows that $(\nabla \phi) P_n B P_n \in C_c(\mathbb{R}^d, S^d(H))$. Hence, there is a constant C independent of m , such that

$$\left\| v^E((1-\phi)K_m P_n B K_m P_n)(x) \right\|_{S^d(H)} \leq C \langle x \rangle^{-1-\eta},$$

where v is a vector field, $\eta \geq 0$, and $\eta = \varepsilon$ for $v = \partial_R$. Thus,

$$\left\| \bigwedge_{j=0}^{d-1} ((dA_{\phi,n,m})e^{-su_j A_{\phi,n,m}^2})(x) \right\|_{S^1(H)} \leq C^d \langle x \rangle^{-d-\varepsilon} dx,$$

which is integrable on $\mathbb{R}^d \times \Delta_{d-1}$, which allows us to take the limit $m \rightarrow \infty$ under the integral.

For the last limit $n \rightarrow \infty$, we partition Δ_{d-1} via

$$\Delta_{d-1} = \bigcup_{k=0}^{d-1} M_k = \dot{\bigcup}_{k=0}^{d-1} N_k,$$

where $M_k := \{u \in \Delta_{d-1}, u_k \geq \frac{1}{d}\}$, $N_k := M_k \setminus (\bigcup_{l=0}^{k-1} M_l)$. For $u \in N_k$, we have by Hypothesis 2.12 a constant C independent of n , such that, for $t > 0$,

$$\begin{aligned} & \left\| \bigwedge_{j=0}^{d-1} ((dA_{\phi,n})e^{-su_j A_{\phi,n}^2})(x) \right\|_{S^1(H)} \\ & \leq C \prod_{j=0}^{d-1} \tau^{\alpha, \beta_j, v_j, d, \delta_j}((1-\phi)B) \sup_{\lambda \in \mathbb{R}} (\langle \lambda \rangle^{-d\alpha} e^{-tu_k \lambda^2}) \langle x \rangle^{-d-\varepsilon} dx, \end{aligned}$$

where $\beta_j = j\alpha$, $v_j = \nabla$ for $j \neq k$, $v_k = \partial_R$, and $\delta_j = 1$ for $j \neq k$, and $\delta_k = 1 + \varepsilon$. In the estimate, we used the fact that P_n commutes with A_0 , and, as seen before, that $\langle A_0 \rangle^{-\alpha+\beta_j} (v_j \phi) B \langle A_0 \rangle^{-\beta_j} \in C_c(\mathbb{R}^d, S^d(H))$, which implies that the involved seminorms $\tau^\bullet((1-\phi)B)$ are finite. We may interchange the limit $n \rightarrow \infty$ with the trace and the integrals in (81) and obtain the claimed formula (77). ■

If the one-forms dA admit radial limits, we may pass to these limits in the above trace formula.

Corollary 6.5. Assume Hypothesis 2.12, and denote $A^\circ(y)\psi := \lim_{R \rightarrow \infty} A(Ry)\psi$, for $\psi \in \text{Dom } A_0$, and $y \in S_1(0)$. Assume that $A^\circ\psi$ is differentiable on $S_1(0)$ for $\psi \in \text{Dom } A_0$, such that for a.e. $y \in S_1(0)$,

$$\lim_{R \rightarrow \infty} R \|\partial_i A^\circ(y)\psi - \partial_i A(Ry)\psi\|_H = 0, \quad (82)$$

and that for $\beta \in [-2N + \alpha, 2N + 1]$, and all unit vector fields v in $TS_1(0)$,

$$\langle A_0 \rangle^{-\alpha+\beta} (vA^\circ) \langle A_0 \rangle^{-\beta} \in L^\infty(S_1(0), S^d(H)). \quad (83)$$

Denote, for $\rho \in C_c^\infty(\mathbb{R})$,

$$\widetilde{A}_\rho^\circ(x) := A_0 + (1 - \rho(|x|)) \left(A^\circ \left(\frac{x}{|x|} \right) - A_0 \right).$$

Then, for $t > 0$, and any $\rho \in C_c^\infty(\mathbb{R})$, with $\rho \equiv 1$ near 0,

$$\begin{aligned} & \text{tr}_{L^2(\mathbb{R}^d, H)} \text{tr}_{\mathbb{C}^r} (e^{-tD^*D} - e^{-tDD^*}) \\ &= \frac{2}{d} (4\pi)^{-\frac{d}{2}} i^d \kappa_c t^{\frac{d}{2}} \int_{s \in \Delta_{d-1}} \int_{\mathbb{R}^d} \text{tr}_H \bigwedge_{j=0}^{d-1} ((d\widetilde{A}_\rho^\circ) e^{-ts_j \widetilde{A}_\rho^{\circ 2}}) du. \end{aligned}$$

Proof. We first note that A° is well defined. Indeed, for a.e. $y \in S_1(0)$,

$$A(Ry) - A(0) = \int_0^R (\partial_R A)(sy) ds,$$

and by Hypothesis 2.12, there is a constant C , such that, for $\beta \in [-2N + \alpha, 2N + 1]$,

$$\|\langle A_0 \rangle^{-\alpha+\beta} (\partial_R A)(sy) \langle A_0 \rangle^{-\beta}\|_{S^d(H)} \leq C \langle s \rangle^{-1-\varepsilon},$$

which is integrable on $s \in (0, \infty)$. Moreover, we estimate for $y \in S_1(0)$, and $k \in [-2N, 2N]$ by Hypothesis 2.12,

$$\begin{aligned} & \|\langle A_0 \rangle^k (A^\circ(y) - A_0) \langle A_0 \rangle^{-k} \langle A_0 \rangle_z^{-1}\|_{B(H)} \\ & \leq \sup_{x \in \mathbb{R}^d} \|\langle A_0 \rangle^k (A(x) - A_0) \langle A_0 \rangle^{-k} \langle A_0 \rangle_z^{-1}\|_{B(H)} \xrightarrow{z \rightarrow \infty} 0, \end{aligned} \quad (84)$$

which implies that $A^\circ(y)$ is self-adjoint on $\text{Dom } A_0$ and that $\text{Dom}(A^\circ(y))^k = \text{Dom } A_0^k$, for $k \in [0, 2N]$, and that the graph norms are equivalent, uniformly in $y \in S_1(0)$ by Kato–Rellich. Similarly, we introduce for $n, m \in \mathbb{N}$, $\rho \in C_c^\infty(\mathbb{R})$,

$$\widetilde{A}_{n,m,l,\rho}^\circ := A_0 + \delta_l(K_m P_n (\widetilde{A}_\rho^\circ - A_0) P_n K_m).$$

Analogously to (84), we conclude that the graph norms of $\widetilde{A}_{n,m,l,\rho}^{\circ k}$ and A_0^k are equivalent, uniformly in $n, m, l \in \mathbb{N}$ for $k \in [0, 2N]$. In the proof of Theorem 6.4, we replace, due to the limit $R \rightarrow \infty$, in (79), the terms A_* by $\widetilde{A}_{n,m,l,\rho}^\circ$ and dA_* by $d\widetilde{A}_{n,m,l,\rho}^\circ$, which follows from the additional condition (82), and dominated convergence after scaling coordinates from $S_R(0)$ to $S_1(0)$. The presence of K_m ensures that the limit $R \rightarrow \infty$ of the integrand is still in trace-class. We now proceed similarly to the proof of Theorem 6.4 and obtain

$$\begin{aligned} & \text{tr}_{L^2(\mathbb{R}^d, H)} \text{tr}_{\mathbb{C}^r} (e^{-tD^*D} - e^{-tDD^*}) \\ &= \lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} \lim_{l \rightarrow \infty} \frac{2}{d} (4\pi)^{-\frac{d}{2}} i^d \kappa_c t^{\frac{d}{2}} \\ & \quad \times \int_{s \in \Delta_{d-1}} \int_{\mathbb{R}^d} \text{tr}_H \bigwedge_{j=0}^{d-1} ((d\widetilde{A}_{n,m,l,\rho}^\circ) e^{-ts_j \widetilde{A}_{n,m,l,\rho}^{\circ 2}}) d\mathcal{U}. \end{aligned}$$

It remains to evaluate the iterated limits $n, m, l \rightarrow \infty$. Since the graph norms of the powers of $\widetilde{A}_{n,m,l,\rho}^\circ$ are uniformly equivalent to those of A_0 , the limiting procedure is similar to the one in the proof of Theorem 6.4, if we show that the operator family $\widetilde{A}_\rho^\circ$ satisfies, for $\beta \in [-2N + \alpha, 2N + 1]$,

$$\begin{aligned} & \tau^{\alpha, \beta, \nabla, d, 1}(\widetilde{A}_\rho^\circ - A_0) < \infty, \\ & \exists \varepsilon > 0 : \tau^{\alpha, \beta, \partial_R, d, 1+\varepsilon}(\widetilde{A}_\rho^\circ - A_0) < \infty. \end{aligned} \tag{85}$$

Indeed, by (83), we have a constant C , such that

$$\left\| \langle A_0 \rangle^{-\alpha+\beta} \left(A^\circ \left(\frac{x}{|x|} \right) - A_0 \right) \langle A_0 \rangle^{-\beta} \right\|_{S^d(H)} \leq C.$$

The fact that ρ' is compactly supported, and condition (83), are implied by direct calculation (85) for any choice of $\varepsilon > 0$. ■

7. Applications

The principal trace formulas displayed in Theorem 6.4 and in Corollary 6.5 enable us to establish a condition of the existence and a formula for the index of D . At this stage, we introduce the following regularized notion of an index, which might

still exist even if D fails to be Fredholm, which is called the (partial) Witten index. Without the presence of the partial trace, its notion was introduced in [26].

Definition 7.1. Let T be a linear, densely defined operator on $\mathbb{C}^r \otimes X$ for some separable complex Hilbert space X . We say the partial (semi-group regularized) Witten index of T exists, if for some $t_0 > 0$,

$$\mathrm{tr}_{\mathbb{C}^r}(e^{-tT^*T} - e^{-tTT^*}) \in S^1(X), \quad t \geq t_0,$$

and if the limit

$$\mathrm{ind}_W T := \lim_{t \rightarrow \infty} \mathrm{tr}_X(\mathrm{tr}_{\mathbb{C}^r}(e^{-tT^*T} - e^{-tTT^*}))$$

exists. Then, $\mathrm{ind}_W T$ is called the partial Witten index of T .

Remark 7.2. Similar to the proof of [13, Lemma 1], one obtains the analogous result for the partial Witten index. Namely, if for some $t_0 > 0$, the condition

$$\mathrm{tr}_{\mathbb{C}^r}(e^{-tT^*T} - e^{-tTT^*}) \in S^1(X), \quad t \geq t_0,$$

holds, and T is additionally Fredholm, then T admits a partial Witten index, $\mathrm{ind}_W T$, which coincides with the Fredholm index $\mathrm{ind} T = \dim \ker T - \dim \mathrm{coker} T$.

It is clear that $\mathrm{ind}_W D$ exists, whenever the right-hand sides of the principal trace formulas in Theorem 6.4 or Corollary 6.5 admit a limit for $t \rightarrow \infty$. If D is Fredholm, this is the case by Remark 7.2. However, for the interesting case where D is non-Fredholm, we also present an example for which the Witten index exists, and can be calculated directly in terms of its symbol. We start with the Fredholm result first.

Theorem 7.3. Assume Hypothesis 2.12. Additionally, assume that there exists $R_0 \geq 0$, such that, for $|x| \geq R_0$, we have $0 \in \rho(A(x))$. Then, D is Fredholm, and the Fredholm index $\mathrm{ind} D$ is given by

$$\mathrm{ind}_W D = \frac{2}{d}(4\pi)^{-\frac{d}{2}} i^d \kappa_c \lim_{t \rightarrow \infty} t^{\frac{d}{2}} \int_{s \in \Delta_{d-1}} \int_{\mathbb{R}^d} \mathrm{tr}_H \bigwedge_{j=0}^{d-1} ((dA_\phi) e^{-ts_j A_\phi^2}) ds, \quad (86)$$

where $A_\phi := A_0 + (1 - \phi)(A - A_0)$ for any $\phi \in C_c^\infty(\mathbb{R}^d)$, and the formula is independent of the choice of ϕ .

Proof. If D is Fredholm, D admits a partial Witten index, according to Remark 7.2, and it equals the right-hand side of (86) by Theorem 6.4. We, thus, only need to show that D is Fredholm. Since $A(x)$ is invertible for $|x|$ large enough, let $C > 0$ be a constant such that $A(x)^2 \geq C$ for $|x| \geq R_0$. Note that $D^*D = \Delta + A^2 - i(\not{D}B)$ as

differential operator. On the domain of D^*D , we thus have some constant C' , such that

$$D^*D \geq \Delta + C - \frac{C'}{\langle X \rangle}, \quad (87)$$

where we used the fact that $A^2 \geq 0$, and $i(\not\partial B)$ is bounded and decays like $|x|^{-1}$ for $|x| \rightarrow \infty$. By Seeley's theorem [13, Theorem 1], the elliptic differential operator $\Delta + C - \frac{C'}{\langle X \rangle}$ is Fredholm. The operator inequality (87) then implies that D^*D is also Fredholm. The analogous argument works for DD^* as well; hence, D is Fredholm. ■

The following examples are presented in more detail in [23]; here, we merely quote the results without the proofs. The basic object is a Dirac–Schrödinger operator D_V which is non-Fredholm.

Definition 7.4. For a potential $V : \mathbb{R}^d \times \mathbb{R} \rightarrow B_{sa}(H)$, define the associated *massless* $(d + 1)$ -Dirac–Schrödinger operator D_V ,

$$\begin{aligned} (D_V f)(x, y) &:= i \sum_{j=1}^d c^j \partial_{x^j} f(x, y) + i \partial_y f(x, y) + V(x, y) f(x, y), \\ x &\in \mathbb{R}^d, \quad y \in \mathbb{R}, \\ f &\in W^{1,2}(\mathbb{R}^{d+1}, \mathbb{C}^r \otimes H). \end{aligned}$$

Example 7.5 ([23, Theorem 1.1]). Let $V \in C_b^2(\mathbb{R}^d \times \mathbb{R}, B_{sa}(H))$, where $B_{sa}(H)$ is equipped with the strong operator topology. Assume furthermore that, for $i \in \{1, \dots, d\}$ and $k \in \{0, 1, 2\}$,

$$\begin{aligned} \|y \mapsto \partial_{x^i} \partial_y^k V(x, y)\|_{L^d(\mathbb{R}, S^d(H))} &= O(|x|^{-1}), \quad |x| \rightarrow \infty, \\ \exists \varepsilon > 0 : \|y \mapsto \partial_R \partial_y^k V(x, y)\|_{L^d(\mathbb{R}, S^d(H))} &= O(|x|^{-1-\varepsilon}), \quad |x| \rightarrow \infty, \end{aligned}$$

and that for any $\hat{x} \in S_1(0)$, $x_0 \in \mathbb{R}^d$, and $\gamma \in \mathbb{N}_0^d$ with $|\gamma| \leq 1$, we have

$$\lim_{R \rightarrow \infty} R^{|\gamma|} \|(\partial_x^\gamma V)(x_0 + R\hat{x}, \cdot) - (\partial_x^\gamma V)(R\hat{x}, \cdot)\|_{L^\infty(\mathbb{R}, B(H))} = 0.$$

Then,

$$\text{ind}_W D_V = \frac{1}{2\pi} (4\pi)^{-\frac{d-1}{2}} \frac{(\frac{d-1}{2})!}{d!} \kappa_c \int_{\mathbb{R}^d} \text{tr}_H ((U^V)^{-1} dU^V)^{\wedge d},$$

where $\wedge d$ is the d -fold exterior power,

$$\kappa_c := \text{tr}_{\mathbb{C}^r} (c^1 \cdot \dots \cdot c^d),$$

and the unitary U^V is given by

$$U^V(x) := \lim_{n \rightarrow \infty} U^{V(x, \cdot)}(n, -n), \quad x \in \mathbb{R}^d,$$

where $U^A(y_1, y_2)$, $y_1, y_2 \in \mathbb{R}$, for a given $A : \mathbb{R} \rightarrow B_{sa}(H)$, is the (unique) evolutions system of the equation

$$u'(y) = iA(y)u(y), \quad y \in \mathbb{R},$$

i.e., for $y, y_1, y_2, y_3 \in \mathbb{R}$,

$$\begin{aligned} \partial_{y_1} U^A(y_1, y_2) &= iA(y_1)U^A(y_1, y_2), \\ \partial_{y_2} U^A(y_1, y_2) &= -iU^A(y_1, y_2)A(y_2), \\ U^A(y_1, y_2)U^A(y_2, y_3) &= U^A(y_1, y_3), \\ U^A(y, y) &= 1_H. \end{aligned}$$

With the minimal choice $r = 2^{\frac{d-1}{2}}$, and sign convention⁴

$$\kappa_c = l(-i)^d (2i)^{\frac{d-1}{2}},$$

we have

$$\text{ind}_W D_V = (2\pi i)^{-\frac{d+1}{2}} \frac{(\frac{d-1}{2})!}{d!} \int_{\mathbb{R}^d} \text{tr}_H((U^V)^{-1} dU^V)^{\wedge d}.$$

This formula generalizes an index formula found in [7, 14, 16] for the case $d = 1$ to $d \geq 3$ odd. For a special choice of the potential V , the index formula becomes even more concrete. We will close the paper with this example.

Definition 7.6. Let $F : \mathbb{R}^d \rightarrow \mathbb{R}^d$ be a bounded smooth function with bounded derivatives, such that

$$\begin{aligned} \partial_{x_i} F(x) &= O(|x|^{-1}), \quad |x| \rightarrow \infty, \\ \exists \varepsilon > 0 : \partial_R F(x) &= O(|x|^{-1-\varepsilon}), \quad |x| \rightarrow \infty, \end{aligned}$$

and that for any $\hat{x} \in S_1(0)$, $x_0 \in \mathbb{R}^d$, and $\gamma \in \mathbb{N}_0^d$ with $|\gamma| \leq 1$,

$$\lim_{R \rightarrow \infty} R^{|\gamma|} |(\partial^\gamma F)(x_0 + R\hat{x}) - (\partial^\gamma F)(R\hat{x})| = 0.$$

Set $V(x, y) := i \sum_{j=1}^d c^j F_j(x) \phi(y)$, $x \in \mathbb{R}^d$, $y \in \mathbb{R}$, for some function $\phi \in C_c^\infty(\mathbb{R})$ with $\int_{\mathbb{R}} \phi(y) dy = 1$.

⁴This corresponds to the choice $c^j = -i\sigma^j$, where σ^j are classical Pauli matrices.

Example 7.7 ([23, Proposition 1.2]). With V as in Definition 7.6, with the minimal choices $\text{rank}(c^i) = 2^{\frac{d-1}{2}}$ and sign convention $\kappa_c = l(-i)^d (2i)^{\frac{d-1}{2}}$, the partial Witten index of D_V exists, and

$$\text{ind}_W D_V = (2\pi)^{-\frac{d+1}{2}} \frac{(\frac{d-1}{2})!}{d} \int_{\mathbb{R}^d} \frac{(|F| + d - 1)(\cos(2|F|) - 1)^{\frac{d-1}{2}}}{|F|^d} \det DF \, dx,$$

where DF is the Jacobian of F . Note that the integrand extends continuously to $F=0$.

The above formula allows one to show that ind_W may assume any real number for this class of operators D_V if one chooses appropriate diffeomorphisms of $\mathbb{R}^d$ onto balls centred around 0 for the function F (cf. [23, Corollary 4.6]).

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References

- [1] N. Anghel, L^2 -index formulae for perturbed Dirac operators. *Comm. Math. Phys.* **128** (1990), no. 1, 77–97 Zbl 0697.58048 MR 1042444
- [2] N. Anghel, On the index of Callias-type operators. *Geom. Funct. Anal.* **3** (1993), no. 5, 431–438 Zbl 0843.58116 MR 1233861
- [3] M. F. Atiyah, V. K. Patodi, and I. M. Singer, Spectral asymmetry and Riemannian geometry. I. *Math. Proc. Cambridge Philos. Soc.* **77** (1975), 43–69 Zbl 0297.58008 MR 0397797
- [4] M. F. Atiyah, V. K. Patodi, and I. M. Singer, Spectral asymmetry and Riemannian geometry. II. *Math. Proc. Cambridge Philos. Soc.* **78** (1975), no. 3, 405–432 Zbl 0314.58016 MR 0397798
- [5] M. F. Atiyah, V. K. Patodi, and I. M. Singer, Spectral asymmetry and Riemannian geometry. III. *Math. Proc. Cambridge Philos. Soc.* **79** (1976), no. 1, 71–99 Zbl 0325.58015 MR 0397799
- [6] N. Berline, E. Getzler, and M. Vergne, *Heat kernels and Dirac operators*. Grundlehren Math. Wiss. 298, Springer, Berlin, 1992 Zbl 0744.58001 MR 1215720
- [7] D. Bollé, F. Gesztesy, H. Grosse, W. Schweiger, and B. Simon, Witten index, axial anomaly, and Kreĭn’s spectral shift function in supersymmetric quantum mechanics. *J. Math. Phys.* **28** (1987), no. 7, 1512–1525 Zbl 0643.47005 MR 0894842
- [8] R. Bott and R. Seeley, Some remarks on the paper of Callias: “Axial anomalies and index theorems on open spaces”. *Comm. Math. Phys.* **62** (1978), no. 3, 235–245 Zbl 0409.58019 MR 0507781
- [9] M. Braverman and P. Shi, Cobordism invariance of the index of Callias-type operators. *Comm. Partial Differential Equations* **41** (2016), no. 8, 1183–1203 Zbl 1374.19001 MR 3532391

- [10] J. Brüning and H. Moscovici, [\$L^2\$ -index for certain Dirac–Schrödinger operators](#). *Duke Math. J.* **66** (1992), no. 2, 311–336 Zbl 0765.58029 MR 1162192
- [11] J. Brüning and R. Seeley, [The resolvent expansion for second order regular singular operators](#). *J. Funct. Anal.* **73** (1987), no. 2, 369–429 Zbl 0625.47040 MR 0899656
- [12] U. Bunke, [A \$K\$ -theoretic relative index theorem and Callias-type Dirac operators](#). *Math. Ann.* **303** (1995), no. 2, 241–279 Zbl 0835.58035 MR 1348799
- [13] C. Callias, [Axial anomalies and index theorems on open spaces](#). *Comm. Math. Phys.* **62** (1978), no. 3, 213–234 Zbl 0416.58024 MR 0507780
- [14] A. Carey, F. Gesztesy, H. Grosse, G. Levitina, D. Potapov, F. Sukochev, and D. Zanin, [Trace formulas for a class of non-Fredholm operators: A review](#). *Rev. Math. Phys.* **28** (2016), no. 10, article no. 1630002 Zbl 1394.47023 MR 3572626
- [15] A. Carey, F. Gesztesy, G. Levitina, R. Nichols, F. Sukochev, and D. Zanin, [The limiting absorption principle for massless Dirac operators, properties of spectral shift functions, and an application to the Witten index of non-Fredholm operators](#). Mem. Eur. Math. Soc. 4, European Mathematical Society, Berlin, 2023 Zbl 1529.81006 MR 4601596
- [16] A. Carey, F. Gesztesy, G. Levitina, D. Potapov, F. Sukochev, and D. Zanin, [On index theory for non-Fredholm operators: A \$\(1 + 1\)\$ -dimensional example](#). *Math. Nachr.* **289** (2016), no. 5-6, 575–609 Zbl 1384.47006 MR 3486146
- [17] A. Carey, F. Gesztesy, G. Levitina, and F. Sukochev, [The spectral shift function and the Witten index](#). In *Spectral theory and mathematical physics*, pp. 71–105, Oper. Theory Adv. Appl. 254, Birkhäuser, [Cham], 2016 Zbl 6981831 MR 3526446
- [18] A. Carey and G. Levitina, [Index theory beyond the Fredholm case](#). Lecture Notes in Math. 2323, Springer, Cham, 2022 Zbl 1515.58005 MR 4628017
- [19] C. Carvalho and V. Nistor, [An index formula for perturbed Dirac operators on Lie manifolds](#). *J. Geom. Anal.* **24** (2014), no. 4, 1808–1843 Zbl 1331.58028 MR 3261719
- [20] S. Cecchini, [Callias-type operators in \$C^*\$ -algebras and positive scalar curvature on non-compact manifolds](#). *J. Topol. Anal.* **12** (2020), no. 4, 897–939 Zbl 1451.19019 MR 4146567
- [21] J. Dixmier, *C^* -algebras*. North-Holland Math. Libr. 15, North-Holland, Amsterdam, 1977 Zbl 0372.46058 MR 0458185
- [22] O. Fürst, [Trace class properties of resolvents of Callias operators](#). *J. Spectr. Theory* **13** (2023), no. 2, 525–553 Zbl 07761494 MR 4651732
- [23] O. Fürst, [The Witten index of massless \$\(d + 1\)\$ -Dirac–Schrödinger operators](#). *J. Geom. Phys.* **209** (2025), article no. 105413 Zbl 07972452 MR 4844807
- [24] F. Gesztesy, Y. Latushkin, K. A. Makarov, F. Sukochev, and Y. Tomilov, [The index formula and the spectral shift function for relatively trace class perturbations](#). *Adv. Math.* **227** (2011), no. 1, 319–420 Zbl 1220.47017 MR 2782197
- [25] F. Gesztesy, Y. Latushkin, F. Sukochev, and Y. Tomilov, [Some operator bounds employing complex interpolation revisited](#). In *Operator semigroups meet complex analysis, harmonic analysis and mathematical physics*, pp. 213–239, Oper. Theory Adv. Appl. 250, Birkhäuser, Cham, 2015 Zbl 1380.47012 MR 3468218
- [26] F. Gesztesy and B. Simon, [Topological invariance of the Witten index](#). *J. Funct. Anal.* **79** (1988), no. 1, 91–102 Zbl 0649.47012 MR 0950085

- [27] F. Gesztesy and M. Waurick, *The Callias index formula revisited*. Lecture Notes in Math. 2157, Springer, Cham, 2016 Zbl 1359.47001 MR 3497011
- [28] T. Kato, *Perturbation theory for linear operators*. 1980 edn., Classics Math., Springer, Berlin, 1995 Zbl 0435.47001 MR 1335452
- [29] C. Kottke, *A Callias-type index theorem with degenerate potentials*. *Comm. Partial Differential Equations* **40** (2015), no. 2, 219–264 Zbl 1316.58019 MR 3277926
- [30] D. Kucerovsky, *A short proof of an index theorem*. *Proc. Amer. Math. Soc.* **129** (2001), no. 12, 3729–3736 Zbl 0982.58015 MR 1860509
- [31] A. Pushnitski, *The spectral flow, the Fredholm index, and the spectral shift function*. In *Spectral theory of differential operators*, pp. 141–155, Amer. Math. Soc. Transl. Ser. 2 225, American Mathematical Society, Providence, RI, 2008 Zbl 1168.47010 MR 2509781
- [32] J. Råde, *Callias’ index theorem, elliptic boundary conditions, and cutting and gluing*. *Comm. Math. Phys.* **161** (1994), no. 1, 51–61 Zbl 0797.58081 MR 1266069
- [33] J. Robbin and D. Salamon, *The spectral flow and the Maslov index*. *Bull. London Math. Soc.* **27** (1995), no. 1, 1–33 Zbl 0859.58025 MR 1331677
- [34] H. Schulz-Baldes and T. Stoiber, *Callias-type operators associated to spectral triples*. *J. Noncommut. Geom.* **17** (2023), no. 2, 527–572 Zbl 1527.46047 MR 4592880
- [35] P. Shi, *The index of Callias-type operators with Atiyah–Patodi–Singer boundary conditions*. *Ann. Global Anal. Geom.* **52** (2017), no. 4, 465–482 Zbl 1467.58013 MR 3735908
- [36] B. Simon, *Trace ideals and their applications*. 2nd edn., Math. Surveys Monogr. 120, American Mathematical Society, Providence, RI, 2005 Zbl 1074.47001 MR 2154153
- [37] K. van den Dungen, *The index of generalised Dirac–Schrödinger operators*. *J. Spectr. Theory* **9** (2019), no. 4, 1459–1506 Zbl 1439.19008 MR 4033528
- [38] K. van den Dungen, *Generalised Dirac–Schrödinger operators and the Callias theorem*. *Forum Math. Sigma* **13** (2025), article no. e11 Zbl 1567.19002 MR 4854428
- [39] D. R. Yafaev, *Mathematical scattering theory. General theory*. Transl. Math. Monogr. 105, American Mathematical Society, Providence, RI, 1992 Zbl 0761.47001 MR 1180965

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