Trace-class properties of semi-groups associated with operator valued differential operators and their Witten index

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1 Introduction

The central problem we want to discuss is the computation of the trace in $L^2(\mathbb{R}, H)$ of the operator $e^{-tDD^*} - e^{-tD^*D}$ for $D = \partial + A(X)$ and $t > 0$.

Let us begin by outlining the foundational situation, and let us give a summary of the results. We consider a self-adjoint operator A_- in a complex, separable Hilbert space H, which plays the role of a "model operator", more concretely let $A(x)$, $x \in \mathbb{R}$ be a family of self-adjoint operators in H, such that it fulfils the requirements in Definition 2.3 and a selection of conditions from subsection 2.2. Then the operator $A(X)$ in $L^2(\mathbb{R}, H)$ is well-defined by

$$(A(X) f)(x) = A(x) f(x), \text{ for a.e. } x \in \mathbb{R},$$

and for $f \in \mathrm{Dom}(A(X))$, i.e.

$$f \in L^2(\mathbb{R}, H), \ f(x) \in \mathrm{Dom}(A(x)) \text{ for a.e. } x \in \mathbb{R} \text{ and } (x \mapsto A(x) f(x)) \in L^2(\mathbb{R}, H).$$

The conditions on the family $A(x)$, $x \in \mathbb{R}$ imply that A_- is the limit

$$A_- = \lim_{x \to -\infty} A(x),$$

and that also the limiting operator

$$A_+ = \lim_{x \to +\infty} A(x),$$

exists (in a specific sense, c.f. Lemma 2.24). Apart from the possible assumption that A_+ and A_- possess a spectral gap at 0 (cf. Definition 3.8 and Theorem 5.3), there are no further assumptions on the operator A_- (especially a discrete spectrum is not needed).

The new approach, we discuss in this work, is basically that the assumptions made on the family $A(x)$, $x \in \mathbb{R}$ do not imply that $A(x) - A_-$ is necessarily a relative trace-class perturbation of A_-.
Instead, we consider the conditions in Hypothesis A1 (2.10) or Hypothesis A2 (2.11), which are furnished around the semi-group $e^{-tA_-^2}$ generated by A_-^2 and not the resolvent of A_-^2. Befitting the change of perspective from resolvents to semi-groups, the first main results (c.f. Theorem 4.16 and Theorem 4.17) to mention are the trace formulae concerned with the semi-groups of the (non-negative) operators $H_+ = DD^*$ and $H_- = D^*D$ in $L^2(\mathbb{R}, H)$. For $t > 0$ we have,

$$\begin{aligned} \mathrm{tr}_{L^2(\mathbb{R},H)}\left(H_+ e^{-tH_+} - H_- e^{-tH_-}\right) &= (4\pi t)^{-1/2}\, \mathrm{tr}_H\left(A_+ e^{-tA_+^2} - A_- e^{-tA_-^2}\right), \\ \mathrm{tr}_{L^2(\mathbb{R},H)}\left(e^{-tH_+} - e^{-tH_-}\right) &= -\lim_{\epsilon \searrow 0} \mathrm{tr}_H\left(e^{-\epsilon A_-^2}\left(\chi_{t,2\epsilon}(A_+) - \chi_{t,2\epsilon}(A_-)\right) e^{-\epsilon A_-^2}\right), \end{aligned} \tag{1}$$

where for $a, b > 0$ the real function $\chi_{a,b}$ is given by

$$\chi_{a,b}(z) := \frac{e^{bz^2}}{2}\left(\mathrm{erf}\left((a+b)^{1/2} z\right) - \mathrm{erf}\left(b^{1/2} z\right)\right), \tag{2}$$

with erf denoting the Gaussian error function, and

$$\begin{aligned}
D =& \partial + A(X), \text{ Dom}(D) = \text{Dom}(\partial) \cap \text{Dom}\left(\widehat{A_-}\right), \\
(\partial f)(x) =& \frac{\mathrm{d}f}{\mathrm{d}x}(x), \text{ for a.e. } x \in \mathbb{R} \text{ and } f \in \text{Dom}(\partial), \\
\text{Dom}(\partial) =& W^{1,2}(\mathbb{R}, H) \\
=& \left\{ f \in L^2(\mathbb{R}, H), \ f \text{ weakly differentiable in } H, \ f' \in L^2(\mathbb{R}, H) \right\}. \qquad (3)
\end{aligned}$$

The operator $\widehat{A_-}$ in $L^2(\mathbb{R}, H)$ denotes the (constant) point-wise multiplication with the operator A_-.

The trace formulae then imply a version of Pushnitski's formula for the spectral shift function of the pair (H_+, H_-) (c.f. Theorem 5.3),

$$\xi(\lambda, H_+, H_-) = \kappa + \frac{1}{\pi} \int_{-\lambda^{1/2}}^{\lambda^{1/2}} \xi(\mu, A_+, A_-) \left(\lambda - \mu^2\right)^{-1/2} \mathrm{d}\mu, \text{ for a.e. } \lambda > 0, \qquad (4)$$

for a constant $\kappa \in \mathbb{R}$. The functions $\xi(\cdot, H_+, H_-)$ and $\xi(\cdot, A_+, A_-)$ are appropriately defined and normalized[1] spectral shift functions associated to the pairs of self-adjoint operators (H_+, H_-) and (A_+, A_-) respectively, which are given by Definition 3.23 and Proposition 3.6.

If we additionally assume that the operators A_+ and A_- possess a spectral gap at 0 (i.e. they are boundedly invertible in H), we show that the operator D has a well-defined (semi-group regularized) Witten index, $\text{ind}_W(D)$, a weaker result than D being Fredholm, however, which is to be expected for a family $A(x) - A_-$, $x \in \mathbb{R}$, of not even relative compact perturbations of A_-.

Furthermore, the Witten index is equal to the constant $-\kappa$ from formula (4), if the spectral shift function $\xi(\cdot, A_+, A_-)$, defined according to Proposition 3.6, is replaced by the spectral shift function $\eta(\cdot, A_+, A_-)$, defined according to Definition 3.8, and thus

$$\begin{aligned}
&\text{ind}_W(D) := \lim_{t \to +\infty} \text{tr}_{L^2(\mathbb{R}, H)} \left(e^{-tD^*D} - e^{-tDD^*}\right) \\
&= \lim_{t \to +\infty} \lim_{\epsilon \searrow 0} \text{tr}_H \left(e^{-\epsilon A_-^2} \left(\chi_{t,2\epsilon}(A_+) - \chi_{t,2\epsilon}(A_-)\right) e^{-\epsilon A_-^2}\right) = \kappa = \xi(\lambda, H_+, H_-), \qquad (5)
\end{aligned}$$

for some $\delta > 0$ and a.e. $\lambda \in (0, \delta)$ (c.f. Theorem 5.3).

The trace formulae (1), the presented version of Pushnitski's formula (4) and the calculation of the Witten index for families with invertible endpoints A_+ and A_- in (5) are the central results of this work, which will be derived and proven in the following chapters.

Before we give a more detailed summary of the subsequent chapters and subsections, we outline the context and history of the discussed problems.
Differential operators with operator coefficients of the form $D = \partial + A(X)$, where $A(x)$,

[1]The normalization in this work is necessarily different than in [16] and [30], thus the constant κ is not present in the original Pushnitski formula.

$x \in \mathbb{R}$, is a family of first order, elliptic, differential operators on a compact, odd dimensional manifold with asymptotic endpoints $A_\pm$, boundedly invertible, and the family $A(x)$, $x \in \mathbb{R}$, and $A_\pm$ with only discrete spectrum, were discussed by Atiyah, Patodi and Singer in their seminal papers [2], [3], [4], [5]. Particularly the statement that the Fredholm index of D is equal to the spectral flow of the family $A(x)$, $x \in \mathbb{R}$, through 0 was proven and was prominently further discussed by Callias in [11]. An abstraction of this result to a family of self-adjoint operators $A(x)$, $x \in \mathbb{R}$, with constant domain in a separable Hilbert space H was shown by Robbin and Salamon in [34]. Here, the assumption was made that $\operatorname{Dom}(A_-)$ embeds densely and compactly (thus implying pure discrete spectra) into H and that the endpoints $A_\pm$ are boundedly invertible in H.

The results concerned with spectral shift functions of the pairs (H_+, H_-) and (A_+, A_-) respectively, originate from mathematical scattering theory. The spectral shift functions stand in a defining connection with the perturbation determinant D_{H_+/H_-} and D_{A_+/A_-} (cf. [6], [23], [24], [38]), and are the densities in M. G. Krein's famous trace formula (originally presented in [23]),

$$\operatorname{tr}_H (f(A_+) - f(A_-)) = \int_{\mathbb{R}} f'(\mu)\, \xi(\mu, A_+, A_-)\, \mathrm{d}\mu, \tag{6}$$

$\xi(\cdot, A_+, A_-)$ denoting a spectral shift function of the pair (A_+, A_-) and f an appropriate real function. This perspective enables us to discuss the "index=spectral flow"-problem resulting in the formulas (4) and (5).

The first result connecting spectral flow with the Fredholm index was presented in [8]. A formula relating the spectral shift functions of the pairs (H_+, H_-), and (A_+, A_-) respectively, in an abstract operator setting, where the assumption on the discreteness of the spectra of $A_\pm$, $A(x)$, $x \in \mathbb{R}$, was suspended, and also reproducing in this setting the connection of spectral flow with the Fredholm index, is due to Pushnitski in [30]. Therein, Pushnitski essentially replaced the discreteness of the spectra with a trace-class assumption on the family of derivatives $A'(x)$, $x \in \mathbb{R}$, i.e.

$$\int_{\mathbb{R}} \left\| A'(x) \right\|_{S^1(H)} \mathrm{d}x < \infty, \tag{7}$$

while A_-, the "model operator", is an arbitrary self-adjoint operator in H. Under this assumption, it is shown that D is Fredholm and

$$\operatorname{ind}(D) = \xi(0, H_+, H_-) = \xi(0, A_+, A_-). \tag{8}$$

Central to this result is the proof of the trace formula (coined Pushnitski formula by some authors, the formula was first presented in the version of a finite dimensional Hilbert space H by Callias in [11]),

$$\operatorname{tr}_{L^2(\mathbb{R},H)} \left((H_+ - z)^{-1} - (H_- - z)^{-1} \right) = \frac{1}{2z} \operatorname{tr}_H \left(A_+ \left(A_+^2 - z\right)^{-1/2} - A_- \left(A_-^2 - z\right)^{-1/2} \right), \tag{9}$$

for $z \in \mathbb{C}\setminus [0,+\infty)$, and the thereof derived formula connecting the spectral shift functions,

$$\xi(\lambda, H_+, H_-) = \frac{1}{\pi}\int_{-\lambda^{1/2}}^{\lambda^{1/2}} \xi(\mu)\left(\lambda-\mu^2\right)^{-1/2} \mathrm{d}\mu, \text{ for a.e. } \lambda > 0. \tag{10}$$

After this breakthrough in [30] getting rid of the condition of discrete spectra, Pushnitski's results were generalized by Gesztesy, Latushkin, Makarov, Sukochev and Tomilov in [16], which is the principal inspiration of this work.

The presence of resolvents in the trace formula (9) already suggests that a setting in which one deals with relative trace-class perturbations, instead of the essential condition (7), is desirable. This goal was achieved in [16], where the essential condition, taking the place of (7), is

$$\int_{\mathbb{R}} \left\| A'(x)\left(A_-^2+1\right)^{-1/2}\right\|_{S^1(H)} < \infty. \tag{11}$$

Furthermore, there are several minor conditions imposed on the family $A(x)$, $x \in \mathbb{R}$, mainly concerned with (domain) properties of the operators $A(x)$, $x \in \mathbb{R}$, and measurability and differentiability of the families $A(x)$, $x \in \mathbb{R}$, and $A'(x)$, $x \in \mathbb{R}$, in a specific sense. All these secondary conditions are implicitly satisfied in the setting of Pushnitski [30], but must be additionally assumed in [16], to ensure the well-definedness of several investigated operators and their domains in this unbounded setup.

Under these conditions and the essential condition (11), the authors of [16] were able to show the trace formula (9) and Pushnitski's formula (10), albeit with the minor effect that the spectral shift functions $\xi(\cdot, H_+, H_-)$ and $\xi(\cdot, A_+, A_-)$ are no longer (Lebesgue-)integrable functions, but are integrable with respect to an appropriate density function times the Lebesgue measure on $\mathbb{R}$. If we assume that A_+ and A_- are boundedly invertible in H, it is also shown that D is Fredholm and the index formula (8) is generalized to the result

$$\begin{aligned}
\operatorname{ind}(D) &= \operatorname{SpFlow}\left((A(x))_{x\in\mathbb{R}}\right) \\
&= \lim_{\epsilon\searrow 0} \xi(\epsilon, H_+, H_-) \\
&= \xi(0, A_+, A_-) \\
&= \operatorname{ind}\left(E_{A_-}((-\infty,0)),\ E_{A_+}((-\infty,0))\right) \\
&= \operatorname{tr}_H\left(E_{A_-}((-\infty,0)) - E_{A_+}((-\infty,0))\right) \\
&= \pi^{-1}\lim_{\epsilon\searrow 0} \Im\left(\log\left(\det{}_H\left((A_+ - \mathbb{i}\epsilon)(A_- - \mathbb{i}\epsilon)^{-1}\right)\right)\right),
\end{aligned} \tag{12}$$

with a choice of branch of $\log(\det{}_H(\cdot))$ on $\{z \in \mathbb{C},\ \Im(z) > 0\}$, according to (14). It is also shown that

$$\xi(\mu, A_+, A_-) = \pi^{-1}\lim_{\epsilon\searrow 0}\Im\left(\log\left(\det{}_H\left((A_+ - \mu - \mathbb{i}\epsilon)(A_- - \mu - \mathbb{i}\epsilon)^{-1}\right)\right)\right), \tag{13}$$

for a.e. $\mu \in \mathbb{R}$, where the branch of $\log(\det{}_H(\cdot))$ on $\{z \in \mathbb{C},\ \Im(z) > 0\}$ is chosen such that

$$\lim_{\Im(z)\to+\infty} \log\left(\det{}_H\left((A_+ - z)(A_- - z)^{-1}\right)\right) = 0. \tag{14}$$

Therefore, the work [16], especially in view of the trace formula (9), gives a complete discussion of a general setup in which the right hand side of (9) is still sensible, and thus exhausts the validity of the trace formula, which compares the resolvents of H_+ and H_-. It should also be noted that in the survey paper [12] by Carey, Gesztesy, Levitina and Sukochev, the results of [16] were put in relation to the (resolvent-regularized) Witten index.

The goal of this work is, roughly speaking, a change of perspective from resolvents as central objects to semi-groups. Therefore our essential conditions describing the trace-class nature of the family $A(x)$, $x \in \mathbb{R}$ are encoded in Hypothesis A1 (2.10) and Hypothesis A2 (2.11). They take the form

$$f(t,s) := \int_{\mathbb{R}} \left\| e^{-tA_-^2} A'(x)\, e^{-sA_-^2} \right\|_{S^1(H)} \mathrm{d}x, \;\; t,s > 0,$$
$$f \in \begin{cases} I^{log}_{-1/4,-1/4}, & \text{for Hypothesis A1,} \\ I^{log}_{-3/4,-1/4} \cap I^{log}_{-1/4,-3/4}, & \text{for Hypothesis A2,} \end{cases} \tag{15}$$

where $\left(f : (0,+\infty)^2 \to \mathbb{R}^{\geq 0}\right) \in I^{log}_{a,b}$, if and only if for all $t_0 > 0$,

$$\int_0^{t_0} \int_0^{t_0} \log(t) \log(s)\, t^a s^b f(t,s)\, \mathrm{d}s\; \mathrm{d}t < \infty. \tag{16}$$

A comparison of the Hypotheses will be discussed in subsection 2.2, in particular it is shown that they are both weaker than condition (11). The perturbation $A(x) - A_-$, $x \in \mathbb{R}$, is not even necessarily relatively compact with respect to A_-, which is the basic novelty of the approach of this work.

These weaker requirements, however, come at a price. The first one is to be expected, namely that we get the trace formulae (1), which are weaker than the trace formula (9). Since one might expect from the aforementioned fact that $A(x) - A_-$, $x \in \mathbb{R}$, is not any more relatively compact with respect to A_-, we can not expect that the operator D is in general Fredholm. However, it is shown that under the additional assumption of boundedly invertible $A_\pm$, that the operator D possesses a semi-group regularized Witten index (c.f. [17]), and we obtain the weaker index formula (5), which generalizes the index formula (12). We must also amend the choice of normalization for the spectral shift function $\xi(\cdot, A_+, A_-)$, which yields the additional constant κ in formula (4)[2]. The second prize, one has to pay, is more subtle. In [16], the authors used condition (11) to deduce some technical facts on domains, closedness, and self-adjointness of the involved operators. The Hypotheses A1 (2.10) and A2 (2.10), summarized in (15), do not allow these statements to be made. We therefore have to assume Hypothesis B1 (2.12) or Hypothesis B2 (2.14), which do not carry any additional requirements on the trace-class properties of the family $A(x)$, $x \in \mathbb{R}$, but are in essence Kato-Rellich bounds.

[2] To differentiate the two versions of normalization, we choose the symbol $\eta(\cdot, A_+, A_-)$ in (4) instead of $\xi(\cdot, A_+, A_-)$. The definition of $\eta(\cdot, A_+, A_-)$ is subject of Definition 3.9.

In summary, we are able to weaken the requirements on the family $A(x)$, $x \in \mathbb{R}$, to not relatively compact perturbations, while still retain an interesting trace formula for the difference of semi-groups of $H_\pm$, a formula for the Witten index of D, and a formula for the spectral shift functions of (H_+, H_-) and (A_+, A_-) similar to the Pushnitski formula.

To close this introduction, let us give a syllabus of the chapters and the principal results therein.

1.1 Summary of the chapters

In chapter 2 the precise setting and the assumptions made in this work are presented. Subsection 2.1 introduces the family $A(x)$, $x \in \mathbb{R}$, and the operator A_- more thoroughly, and also fixes notational conventions, which we will use throughout this work. Subsection 2.2 formulates the additional conditions on the family $A(x)$, $x \in \mathbb{R}$, and discusses them, also in comparison to the assumptions in [16], and demonstrate their viability in an example. In the following subsection 2.3 we present certain classical, well-known operator norm inequalities, and prove them by complex interpolation in a self contained manner. In subsection 2.4 we give the first basic results concerned with the operators $H_\pm$ and D, which deal mostly with issues of domain, closedness, normality, and self-adjointness. The final subsection 2.5 of chapter 2 can be considered as the "engine room", containing all technical facts, which are needed, but do not fit in the other chapters. Among them are some integral formulas and some basic facts on Bochner integrability and N-measurability (c.f. [29]).

Chapter 3 contains the proofs of several trace-class memberships of operators in H and $L^2(\mathbb{R}, H)$. Also the spectral shift functions of the pairs (A_+, A_-) and (H_+, H_-) are constructed. In the first subsection 3.1 we show that certain operators, derived from the family $A(x)$, $x \in \mathbb{R}$, are trace-class operators in H, for example if Hypothesis A2 (2.11) holds, we have (c.f. Lemma 3.3)

$$\begin{aligned}
&\left(1 + A_-^2\right)^{-1/4} \left(A(x) - A_-\right) \left(1 + A_-^2\right)^{-3/4} \in S^1(H), \ x \in \mathbb{R} \cup \{\pm\infty\} \\
&\left(1 + A_-^2\right)^{-3/4} \left(A(x) - A_-\right) \left(1 + A_-^2\right)^{-1/4} \in S^1(H), \ x \in \mathbb{R} \cup \{\pm\infty\}. \qquad (17)
\end{aligned}$$

Furthermore, we give estimates of their trace-norms. These memberships allow us to construct spectral shift functions of the pair (A_+, A_-) in the ensuing subsection 3.2. Here, we get different versions (and integrability properties) of spectral shift functions based on the choice of Hypothesis, and if the operators $A_\pm$ have a spectral gap at 0. In subsection 3.3, the bulk of that chapter, we discuss the trace-class memberships of several operators in $L^2(\mathbb{R}, H)$, among which is the difference $e^{-tH_+} - e^{-tH_-}$. We extensively use Duhamel's formula (sometimes also called Duhamel's principle or Volterra series, c.f. [15]) for the perturbation of semi-groups (c.f. Lemma 2.29) and the tensoriality of Hilbert-Schmidt-operators (c.f. Lemma 3.10). Chapter 3 closes with subsection 3.4, in which we construct the spectral shift function of the pair (H_+, H_-).

In chapter 4 we derive the trace formulae for $t > 0$

$$\begin{aligned} \mathrm{tr}_{L^2(\mathbb{R},H)}\left(H_+e^{-tH_+} - H_-e^{-tH_-}\right) &= (4\pi t)^{-1/2}\,\mathrm{tr}_H\left(A_+e^{-tA_+^2} - A_-e^{-tA_-^2}\right), \\ \mathrm{tr}_{L^2(\mathbb{R},H)}\left(e^{-tH_+} - e^{-tH_-}\right) &= -\lim_{\epsilon\searrow 0}\mathrm{tr}_H\left(e^{-\epsilon A_-^2}\left(\chi_{t,2\epsilon}\left(A_+\right) - \chi_{t,2\epsilon}\left(A_-\right)\right)e^{-\epsilon A_-^2}\right), \end{aligned} \tag{18}$$

which were already presented in the introduction as the principal result of this work. To stress the importance of the "Trace Lemma" by Brüning and Seeley [10], subsection 4.1 is entirely devoted to citing this important tool and laying out the general strategy of proof for the trace formulae in the following subsections. The Trace Lemma provides us with the integral kernel in a specific (operator valued) function space, enabling us to calculate the trace by integrating over the (fibre-wise) trace of the diagonal of this kernel. In the next subsection 4.2 we therefore construct integral kernels of the operators P_t^+ and Q_t^+, which are given by

$$\begin{aligned} P_t^+ = D^*e^{-tH_+},\ Q_t^t &= D^*\gamma\left(tH_+\right), \\ \gamma\left(z\right) &:= \begin{cases} \frac{1-e^{-z}}{z}, & z \neq 0 \\ 1, & z = 0, \end{cases} \end{aligned} \tag{19}$$

and satisfy for $t > 0$ on $\mathrm{Dom}\left(\partial\right) \cap \mathrm{Dom}\left(\widehat{A_-}\right)$,

$$H_+e^{-tH_+} - H_-e^{-tH_-} = \left[\partial, P_t^+\right] + \left[A\left(X\right), P_t^+\right], \tag{20}$$

$$e^{-tH_+} - e^{-tH_-} = -t\left[\partial, Q_t^+\right] - t\left[A\left(X\right), Q_t^+\right]. \tag{21}$$

Since the identities (20) extend, after composition and pre-composition with $e^{-\epsilon\left(-\partial^2+\widehat{A_-^2}\right)}$, $\epsilon > 0$, to identities holding in the trace-class of $L^2\left(\mathbb{R}, H\right)$, if Hypothesis A2 (2.11) is assumed, we may use the Trace Lemma, and, due to the commutators with ∂, the fundamental theorem of calculus, to determine the trace as the trace in H of $\lim_{x\to+\infty} k\left(x,x\right)$ $-\ k\left(-x,-x\right)$, where k are the appropriate integral kernels. In the final subsection 4.3 of chapter 4 we calculate the limits $\lim_{x\to+\infty} k\left(x,x\right)$ and $\lim_{x\to-\infty} k\left(x,x\right)$ of the two relevant integral kernels in connection with P_t^+ and Q_t^+ in the weak operator topology. Since these limits must coincide with the aforementioned limit in the trace class of H, $\lim_{x\to+\infty} k\left(x,x\right) - k\left(-x,-x\right)$, we conclude the trace formulae (18), which closes the chapter.
Finally, chapter 5 presents our version of the Pushnitski formula, which is derived from the trace formulae (18), involving the spectral shift functions of the pairs $\left(A_+, A_-\right)$ and $\left(H_+, H_-\right)$, which were constructed in chapter 3,

$$\xi\left(\lambda, H_+, H_-\right) = \kappa + \frac{1}{\pi}\int_{-\lambda^{1/2}}^{\lambda^{1/2}} \xi\left(\mu, A_+, A_-\right)\left(\lambda - \mu^2\right)^{-1/2}\mathrm{d}\mu,\ \text{for a.e. } \lambda > 0, \tag{22}$$

where the indeterminacy κ is due to the nature of the first trace identity in (18), essentially because the limits $\lim_{z\to\pm\infty} ze^{-tz^2} = 0$, $t > 0$, avoid an opportunity to normalize the spectral shift function of (A_+, A_-) sensibly. This normalization issue can be fixed by assuming a spectral gap at 0 of $A_\pm$, and then the second identity of (18) is used to determine[3] κ to be the Witten index of D, $\mathrm{ind}_W(D)$, in this case, and we close the chapter with the index formula

$$\begin{aligned}\mathrm{ind}_W(D) &:= \lim_{t\to+\infty} \mathrm{tr}_{L^2(\mathbb{R},H)}\left(e^{-tD^*D} - e^{-tDD^*}\right)\\ &= \lim_{t\to+\infty}\lim_{\epsilon\searrow 0} \mathrm{tr}_H\left(e^{-\epsilon A_-^2}\left(\chi_{t,2\epsilon}(A_+) - \chi_{t,2\epsilon}(A_-)\right)e^{-\epsilon A_-^2}\right) = \kappa. \end{aligned} \tag{23}$$

[3]In (22) we replace $\xi(\cdot, A_+, A_-)$ by $\eta(\cdot, A_+, A_-)$, which is constructed with the normalization of the spectral gap assumption (c.f. Definition 3.9). For the rigorous formulation c.f. Theorem 5.3.

2 Preliminaries

The goal of this chapter is to setup the examined operator family $A(x),\ x \in \mathbb{R}$, and the operator A_-, define the operators $D_0, H_0, H_\pm$, and D, and derive basic functional analytic properties of these operators.
The first subsection 2.1 fixes the notation used throughout this work and we introduce the operator D_0 in $L^2(\mathbb{R}, H)$, which plays a central role in the discussion of D as a perturbation of D_0. We also introduce the self-adjoint operator $H_0 = D_0^* D_0$, and discuss its domain. The following subsection 2.2 comprises of the presentation of the additional Hypotheses A1 (2.10) and A2 (2.11), which encode the trace-class assumption on the family $A(x),\ x \in \mathbb{R}$, and the Hypotheses B1 (2.12) and B2 (2.14), which encode the Kato-Rellich-type bounds on the family $A(x),\ x \in \mathbb{R}$. We discuss the significance of these conditions, compare them to the assumptions made in [16], and illustrate the differences in an example. These Hypotheses, especially B1 and B2, allow us in the next subsection 2.4 to introduce the operators D and $H_\pm$ together with a discussion of their domains, showing that D is normal with $\mathrm{Dom}(D^*) = \mathrm{Dom}(D) = \mathrm{Dom}(D_0)$, and that the operators $H_\pm$ are non-negative and self-adjoint on $\mathrm{Dom}(H_\pm) = \mathrm{Dom}(H_0)$. We should emphasize that this whole chapter orients itself largely at the preparatory sections in [16], and mainly presents the necessary amendments.

2.1 Basic Definitions

Let us start with the disclaimer that well-known results, we do not explicitly cite, are contained in any good textbook on analysis and functional analysis (for example [13], [14], [31], [32], [33] or [39]).

Throughout the whole of this work we set H to be a separable, complex Hilbert space. With $\mathbb{i}$ we denote the imaginary unit in $\mathbb{C}$ and with $\Im$ and $\Re$ the imaginary and real part, respectively. Let us further fix the following notations.
$L^2(\mathbb{R})$ denotes the space of Lebesgue square integrable elements over $\mathbb{R}$. We introduce the (separable,) complex Hilbert space $L^2(\mathbb{R}, H)$ as the completion of $L^2(\mathbb{R}) \otimes H$ with respect to the tensor Hilbert product. The induced norm on $L^2(\mathbb{R}, H)$ is equal to the norm $\|\cdot\|_{L^2(\mathbb{R},H)}$, given by

$$\|f\|_{L^2(\mathbb{R},H)}^2 := \int_{\mathbb{R}} \|f(x)\|_H^2 \, \mathrm{d}x, \quad \text{for } f \in L^2(\mathbb{R}, H). \tag{24}$$

Note that by this definition, membership of an element in $L^2(\mathbb{R}, H)$ automatically implies its (Bochner)-measurability (c.f. the measurability theorem of Pettis in [1] or abstractly via tensor products of Banach spaces [35]).
With $B\left(\widetilde{H}\right)$ we shall denote the bounded linear operators in a Hilbert space $\widetilde{H}$.
For the identity in $B\left(\widetilde{H}\right)$ we use[4] the letter 1, and for scalar multiples of the identity operator we use the scalar itself as its symbol (for example $(T - z)^{-1}$, $z > 0$, then denotes

[4]This clash of notation with scalar numbers is always manageable, the correct meaning is clear in all contexts.

the resolvent of T at z).
The domain of an operator T in a Hilbert space $\widetilde{H}$ is denoted by $\mathrm{Dom}(T)$.
If an operator T in a Hilbert space $\widetilde{H}$ is closable, we denote its closure with $\overline{T}$.
If the closure, $\overline{T}$, is furthermore a bounded operator in $\widetilde{H}$ we write $\{T\}$ instead of $\overline{T}$.
With $S^p\left(\widetilde{H}\right)$ we denote the space of Schatten-class operators of order p in a Hilbert space $\widetilde{H}$ and the corresponding norm with

$$\|\cdot\|_{S^p\left(\widetilde{H}\right)}.$$

In particular, S^1 and S^2 denote the trace-class and Hilbert-Schmidt operators respectively, and with $\mathrm{tr}_{\widetilde{H}}$ we denote the trace in $\widetilde{H}$.
We will also use the commonly utilized convention,

$$A \lesssim_I B,$$

if there is a constant $C \geq 0$, only dependent on the variables in the index set I, such that

$$A \leq CB.$$

Finally we use the common abbreviation "a.e." for "almost everywhere" in a measure related context, and use the symbol $\mathbb{1}_M$ for the characteristic function of a (Lebesgue) measurable set M. After we fixed the basic notation, let us introduce some notions central in this work.
Let $B(x)$, $x \in \mathbb{R}$, be a family of (unbounded) operators in H with constant domain $\mathrm{Dom}(B)$. We may define the "vertical multiplication" operator $B(X)$.

Definition 2.1. The domain $\mathrm{Dom}(B(X))$ consists of those elements $g \in L^2(\mathbb{R}, H)$, such that

$$\begin{aligned} g(x) \in \mathrm{Dom}(B(x)), \text{ for a.e. } x \in \mathbb{R}, \\ (y \mapsto B(y)\, g(y)) \in L^2(\mathbb{R}, H). \end{aligned} \tag{25}$$

Then define

$$(B(X) f)(x) := B(x) f(x), \text{ for a.e. } x \in \mathbb{R}, \text{ and } f \in \mathrm{Dom}(B(X)). \tag{26}$$

If B_0 is a fixed operator in H, let us define $\widehat{B_0} := B_0(X)$, the constant vertical multiplication, where $B_0(x) := B_0$, $x \in \mathbb{R}$. We note that, especially if B_0 is closed in H, we have $\mathrm{Dom}\left(\widehat{B_0}\right) = L^2(\mathbb{R}, \mathrm{Dom}(B_0)_\Gamma)$, where $\mathrm{Dom}(B_0)_\Gamma := \left(\mathrm{Dom}(B_0), \|\cdot\|_{\mathrm{Dom}(B_0)}\right)$ with

$$\|\phi\|^2_{\mathrm{Dom}(B_0)} := \|\phi\|^2_H + \|B_0 f\|^2_H, \text{ for } \phi \in H. \tag{27}$$

Clearly, we also have $\mathrm{Dom}\left(\widehat{B_0}\right)_\Gamma = L^2(\mathbb{R}, \mathrm{Dom}(B_0)_\Gamma)$ as Hilbert spaces. It should also be noted that $\widehat{B_0}$ is symmetric (respectively self-adjoint or normal) in $L^2(\mathbb{R}, H)$, if and only if B_0 is symmetric (respectively self-adjoint or normal) in H, which is a simple consequence of Lemma 2.44, since constant operator families are N-measurable (c.f. Definition 2.42).

On $L^2(\mathbb{R}, H)$ we may define the "horizontal derivative" $\partial \equiv \partial_H$.

Definition 2.2. The domain $\mathrm{Dom}(\partial_H)$ consists of those elements $g \in L^2(\mathbb{R}, H)$, such that g is strongly locally absolutely continuous in H, and such that $g' \in L^2(\mathbb{R}, H)$.
Then define

$$(\partial_H f)(x) := f'(x) \text{ for a.e. } x \in \mathbb{R} \text{ and } f \in \mathrm{Dom}(\partial_H). \tag{28}$$

On $L^2(\mathbb{R})$ we use the letter $\partial_{\mathbb{C}}$ to avoid confusion.
We remind us of the usual convention of defining sums and products of unbounded operators A and B, i.e.

$$\begin{aligned} \mathrm{Dom}(A+B) &:= \mathrm{Dom}(A) \cap \mathrm{Dom}(B), \\ (A+B) f &:= Af + Bf, \text{ for } f \in \mathrm{Dom}(A+B), \\ \mathrm{Dom}(AB) &:= \{f \in \mathrm{Dom}(B),\ Bf \in \mathrm{Dom}(A)\}, \\ (AB) f &:= A(Bf), \text{ for } f \in \mathrm{Dom}(AB). \end{aligned} \tag{29}$$

These definitions are in line with the spectral calculus of a self-adjoint operator. We therefore conclude that for a self-adjoint operator B_0 in H we have the following equalities of Hilbert spaces

$$\mathrm{Dom}\left(\widehat{B_0^2}\right)_\Gamma = \mathrm{Dom}\left(\widehat{B_0}^2\right)_\Gamma = L^2\left(\mathbb{R}, \mathrm{Dom}\left(B_0^2\right)_\Gamma\right). \tag{30}$$

Let us now introduce the family of operators $A(x)$, $x \in \mathbb{R}$, and the "model operator" A_- in H.

Definition 2.3. Let A_- be a self-adjoint operator in H with domain $\mathrm{Dom}(A_-)$.
Let $A(x)$, $x \in \mathbb{R}$, be a family of self-adjoint operators in H with $\mathrm{Dom}\left(A(x)^2\right) = \mathrm{Dom}\left(A_-^2\right)$, for $x \in \mathbb{R}$, with

$$\lim_{x \to -\infty} \langle \phi, A(x)\psi \rangle_H = \langle \phi, A_- \psi \rangle_H,\ \phi \in H,\ \psi \in \mathrm{Dom}(A_-). \tag{31}$$

Let $A'(x)$, $x \in \mathbb{R}$, be a family of closed, symmetric operators in H with $\mathrm{Dom}(A'(x)) \supseteq \mathrm{Dom}(A_-)$, $x \in \mathbb{R}$, and such that $A'(x)$ is a continuous, linear operator from $\mathrm{Dom}\left(A_-^2\right)_\Gamma$ to $\mathrm{Dom}(A_-)_\Gamma$ for $x \in \mathbb{R}$. Furthermore, the family $A(x)$, $x \in \mathbb{R}$ is weakly absolutely continuous with derivative $A'(x)$ on $\mathrm{Dom}(A_-)$ and $\mathrm{Dom}\left(A_-^2\right)$, i.e. for all $\phi \in H$ and $\psi \in \mathrm{Dom}(A_-)$, we have

$$\frac{\mathrm{d}}{\mathrm{d}x} \langle \phi, A(x)\psi \rangle_H = \langle \phi, A'(x)\psi \rangle_H, \tag{32}$$

and for all $\phi \in \mathrm{Dom}(A_-)$ and $\psi \in \mathrm{Dom}\left(A_-^2\right)$, we have

$$\frac{\mathrm{d}}{\mathrm{d}x} \langle \phi, A(x)\psi \rangle_{\mathrm{Dom}(A_-)_\Gamma} = \langle \phi, A'(x)\psi \rangle_{\mathrm{Dom}(A_-)_\Gamma}, \tag{33}$$

for a.e. $x \in \mathbb{R}$ and that $A'(x)$ is weakly integrable over $\mathbb{R}$ on $\mathrm{Dom}(A_-)$ and $\mathrm{Dom}\left(A_-^2\right)$, i.e. the above displayed equations (32) and (33) hold in $L^1(\mathbb{R})$, the Lebesgue integrable elements over $\mathbb{R}$. Finally, we require that the families $A(x)$, $x \in \mathbb{R}$, and $A'(x)$, $x \in \mathbb{R}$, are N-measurable (cf. Definition 2.42).

Remark 2.4. A definition and short discussion of the last requirement, i.e. of N-measurability, will be carried out at the end of subsection 2.5 by Definition 2.42 and Lemma 2.44. For the moment, let us note that strong continuity of $A'(\cdot)$ on $\mathrm{Dom}(A_-)$ imply both N-measurabilities.

Let us also introduce the operator D_0 on $L^2(\mathbb{R}, H)$, which is the unperturbed version of D, which we will later define and examine.

Definition 2.5. We define

$$D_0 := \partial + \widehat{A_-}.$$

Clearly D_0 is densely defined, since the dense space $C_c^\infty(\mathbb{R}) \otimes \mathrm{Dom}(A_-)$ is contained in the domain of D_0. To further present the properties of D_0, we cite [16, Lemma 4.2].

Lemma 2.6. *1. The graph norm $\|\cdot\|_{\mathrm{Dom}(D_0)}$ on $\mathrm{Dom}(D_0)_\Gamma$ is equivalent to the norm on $H^1(\mathbb{R}, H) \cap L^2(\mathbb{R}, \mathrm{Dom}(A_-)_\Gamma)$ defined as the maximum of the norms in $H^1(\mathbb{R}, H)$[5] and $L^2(\mathbb{R}, \mathrm{Dom}(A_-)_\Gamma)$; consequently D_0 is closed.*

2. The adjoint D_0^* of the operator D_0 in $L^2(\mathbb{R}, H)$ is given by

$$D_0^* = -\partial + \widehat{A_-}, \quad \mathrm{Dom}(D_0^*) = \mathrm{Dom}(D_0) = \mathrm{Dom}(\partial) \cap \mathrm{Dom}\left(\widehat{A_-}\right). \tag{34}$$

3. The operator D_0 is normal in $L^2(\mathbb{R}, H)$.

4. The spectra of the operators D_0 in $L^2(\mathbb{R}, H)$ and A_- in H satisfy:

$$\sigma(D_0) = \sigma(A_-) + i\mathbb{R}. \tag{35}$$

The proof holds ad verbatim as presented in [16]. Since D_0 is densely defined, closed and normal, we may define the operator H_0 in $L^2(\mathbb{R}, H)$.

Definition 2.7. We define

$$H_0 := D_0^* D_0 = D_0 D_0^*.$$

Since D_0 is closed, we have that H_0 is self-adjoint in $L^2(\mathbb{R}, H)$ and $H_0 \geq 0$. By the general properties of polar decomposition we conclude further that

$$\mathrm{Dom}\left(H_0^{1/2}\right) = \mathrm{Dom}(D_0) = \mathrm{Dom}(D_0^*) = \mathrm{Dom}(\partial) \cap \mathrm{Dom}\left(\widehat{A_-}\right). \tag{36}$$

By using the Fourier transform, we may determine the domain of H_0 more concretely.

[5]Here, $H^1(\mathbb{R}, H)$ denotes the space of locally absolutely continuous H-valued functions over $\mathbb{R}$, with derivative in $L^2(\mathbb{R}, H)$. Put differently, this is the space of first order, H-valued L^2-Sobolev functions over $\mathbb{R}$. Of course $H^1(\mathbb{R}, H) = H^1(\mathbb{R}) \widehat{\otimes} H$, the Hilbert space tensor product of the space of first order L^2-Sobolev functions over $\mathbb{R}$ and H.

Lemma 2.8. *We have*

$$H_0 = -\partial^2 + \widehat{A_-^2}, \tag{37}$$

and particularly

$$\mathrm{Dom}\,(H_0) = \mathrm{Dom}\,(\partial^2) \cap \mathrm{Dom}\left(\widehat{A_-^2}\right). \tag{38}$$

Proof. We first note that for $z \notin \{w \in \mathbb{R},\ w \leq 0\}$ the resolvent $R\,(z, |D_0|)$ of $|D_0|$ is given by

$$(R\,(z, |D_0|)\, f)\,(x) = \frac{1}{2\pi} \int_{\mathbb{R}} \int_{\mathbb{R}} e^{-\mathbb{i}(x-y)\xi} \left(z + \left(A_-^2 + \xi^2\right)^{1/2}\right)^{-1} f\,(y)\,\mathrm{d}y\ \mathrm{d}\xi. \tag{39}$$

Further, for $z \notin \mathbb{R}$ we have for the resolvent $R\,(z, \mathbb{i}\partial)$ of $\mathbb{i}\partial$

$$(R\,(z, \mathbb{i}\partial)\, f)\,(x) = \frac{1}{2\pi} \int_{\mathbb{R}} \int_{\mathbb{R}} e^{-\mathbb{i}(x-y)\xi}\,(z + \xi)^{-1}\, f\,(y)\,\mathrm{d}y\ \mathrm{d}\xi. \tag{40}$$

Therefore, we note that for $z \notin \mathbb{R}$ the resolvents of the operators $|D_0|$, $\mathbb{i}\partial$, and $(\widehat{A_- + z})^{-1}$, the resolvent of $\widehat{A_-}$, mutually commute. Thus, also their spectral projections $E_{|D_0|}$, $E_{\widehat{A_-}}$, and $E_{\mathbb{i}\partial}$ must be mutually commutative, and we obtain a commutative functional calculus of the three operators. For $n \in \mathbb{N}$ put

$$Q_n := E_{\widehat{A_-}}\,([-n, n])\, E_{|D_0|}\,([-n, n])\, E_{\mathbb{i}\partial}\,([-n, n])\,. \tag{41}$$

We note that the functional calculus implies that $J := \bigcup_{n\in\mathbb{N}} \mathrm{rg}\,(Q_n)$ is dense (by the strong convergence of Q_n to 1) in $L^2\,(\mathbb{R}, H)$. For a self-adjoint operator S in H we denote with S_n the sequence of bounded operators given by $S_n := S\mathbb{1}_{[-n,n]}\,(S)$. Thus for $f \in J$ and for $S \in \left\{\widehat{A_-}, \mathbb{i}\partial\right\}$ we have by Lemma 2.6,

$$\begin{aligned}
\left\|S_n^2\,(1 + H_0)^{-1}\, f\right\|_{L^2(\mathbb{R},H)} &= \left\|\left(S_n\,(1 + |D_0|)^{-1}\right)^2 (1 + |D_0|)^2 \left(1 + |D_0|^2\right)^{-1} f\right\|_{L^2(\mathbb{R},H)} \\
&\leq 1^2 \cdot \sup_{\lambda\geq 0} \left|\frac{1 + \lambda^2}{(1 + \lambda)^2}\right| \|f\|_{L^2(\mathbb{R},H)} = \|f\|_{L^2(\mathbb{R},H)}\,.
\end{aligned} \tag{42}$$

Since J is dense in $L^2\,(\mathbb{R}, H)$, the above inequality (42) extends to arbitrary $f \in L^2\,(\mathbb{R}, H)$, also it holds for all $n \in \mathbb{N}$ and therefore in the (strong) limit. Thus we have

$$\left\|(1 + H_0)^{-1}\, f\right\|_{\mathrm{Dom}(\partial^2)\cap\mathrm{Dom}\left(\widehat{A_-^2}\right)} \leq 4\,\|f\|_{L^2(\mathbb{R},H)}\,. \tag{43}$$

This implies $\mathrm{Dom}\,(H_0) \subseteq \mathrm{Dom}\,(\partial^2) \cap \mathrm{Dom}\left(\widehat{A_-^2}\right)$. For $f, g \in \mathrm{Dom}\,(H_0)$ we obtain furthermore

$$\langle \widehat{A_-} f, \partial g\rangle_{L^2(\mathbb{R},H)} = \lim_{m,n\to\infty} \langle \widehat{A_-}_m f, -\mathbb{i}\,(\mathbb{i}\partial)_n\, g\rangle_{L^2(\mathbb{R},H)}$$

$$= -\lim_{m,n\to\infty} \langle -\mathbb{i}\,(\mathbb{i}\partial)_n\, f, \widehat{A_-}_m g\rangle_{L^2(\mathbb{R},H)}$$
$$= -\langle \partial f, \widehat{A_-} g\rangle_{L^2(\mathbb{R},H)}. \tag{44}$$

Consequently we have

$$\begin{aligned}\langle H_0 f, g\rangle_{L^2(\mathbb{R},H)} &= \langle D_0 f, D_0 g\rangle_{L^2(\mathbb{R},H)} = \langle \left(\partial + \widehat{A_-}\right) f, \left(\partial + \widehat{A_-}\right) g\rangle_{L^2(\mathbb{R},H)} \\ &= \langle \partial f, \partial g\rangle_{L^2(\mathbb{R},H)} + \langle \widehat{A_-} f, \widehat{A_-} g\rangle_{L^2(\mathbb{R},H)} \\ &= \langle \left(-\partial^2 + \widehat{A_-^2}\right) f, g\rangle_{L^2(\mathbb{R},H)}. \end{aligned} \tag{45}$$

By the density of $\mathrm{Dom}\,(H_0)$ in $L^2\,(\mathbb{R}, H)$ we conclude

$$H_0 \subseteq -\partial^2 + \widehat{A_-^2}. \tag{46}$$

Since $T_0 := -\partial^2 + \widehat{A_-^2}$ is densely defined, and symmetric we have

$$T_0 \subseteq T_0^* \subseteq H_0^* = H_0 \subseteq T_0, \tag{47}$$

which shows that $T_0 = H_0$. ■

2.2 Hypotheses

After we fixed the basic requirements on the operator A_- and the family $A\,(x)$, $x \in \mathbb{R}$, we may specify their relationship by introducing a trace-class membership and certain integrability conditions. Before we do so, we introduce for convenience the following recurring space of functions.

Definition 2.9. For $\alpha, \beta \in \mathbb{R}$, let $I_{\alpha,\beta}$ denote the space of non-negative, measurable functions $f : (0,\infty)^2 \to [0,\infty)$, such that for all $t_0 > 0$,

$$\int_0^{t_0} \int_0^{t_0} x^\alpha y^\beta f\,(x,y)\,\mathrm{d}y\;\mathrm{d}x < \infty. \tag{48}$$

Let $I_{\alpha,\beta}^{log}$ denote the space of non-negative, measurable functions $f : (0,\infty)^2 \to [0,\infty)$, such that for all $t_0 > 0$,

$$\int_0^{t_0} \int_0^{t_0} x^\alpha \left|\log\,(x)\right| y^\beta \left|\log\,(y)\right| f\,(x,y)\,\mathrm{d}y\;\mathrm{d}x < \infty. \tag{49}$$

Let us specify the trace-class assumptions on the family $A\,(x)$, $x \in \mathbb{R}$. This is the content of the following two Hypotheses A1 (2.10) and A2 (2.11).

Hypothesis 2.10 (Hypothesis A1)**.** We assume that for $s, t > 0$ and a.e. $x \in \mathbb{R}$ the operator

$$e^{-tA_-^2} A'\,(x)\, e^{-sA_-^2}$$

is a trace-class operator in H and that

$$y \mapsto \left\| e^{-tA_-^2} A'(y) \, e^{-sA_-^2} \right\|_{S^1(H)}$$

is integrable over $\mathbb{R}$. Finally we require that

$$\left((u,v) \mapsto \int_{\mathbb{R}} \left\| e^{-uA_-^2} A'(y) \, e^{-vA_-^2} \right\|_{S^1(H)} \mathrm{d}y \right) \in I^{log}_{-1/4,-1/4}. \tag{50}$$

Hypothesis 2.11 (Hypothesis A2)**.** We assume that for $s,t > 0$ and a.e. $x \in \mathbb{R}$, the operator

$$e^{-tA_-^2} A'(x) \, e^{-sA_-^2},$$

is a trace-class operator in H and that

$$y \mapsto \left\| e^{-tA_-^2} A'(y) \, e^{-sA_-^2} \right\|_{S^1(H)},$$

is integrable over $\mathbb{R}$. Finally, we require that

$$\left((u,v) \mapsto \int_{\mathbb{R}} \left\| e^{-uA_-^2} A'(y) \, e^{-vA_-^2} \right\|_{S^1(H)} \mathrm{d}y \right) \in I^{log}_{-3/4,-1/4} \cap I^{log}_{-1/4,-3/4}. \tag{51}$$

It is obvious that Hypothesis A2 (2.11) is stronger than Hypothesis A1 (2.10), however, the distinction of the two is stressed here, since for some parts of this work it is sufficient to just assume Hypothesis A1 (2.10) (e.g. the central Theorem 3.19).

We also need additional assumptions on the uniformity of the family $A(x)$, $x \in \mathbb{R}$. This is owed to the fact that Hypothesis A1 (2.10) and A2 (2.11) do not imply Kato-Rellich bounds on the perturbations $A(x) - A_-$, $x \in \mathbb{R}$, relative to A_- and $D - D_0$ relative to D_0.
Furthermore, Duhamel's formula (cf. Lemma 2.29), which is used extensively in chapter 3, especially subsection 3.3, requires in these settings that the domains of H_+ and H_- coincide with the domain of H_0 (c.f. Definition 2.26), which is another deviation from [16] (the conditions therein justify only $\mathrm{Dom}\,(H_+)^{1/2} = \mathrm{Dom}\,(H_-)^{1/2} = \mathrm{Dom}\,(H_0)^{1/2}$). Thus, while our trace-class assumptions are weaker than in [16], the Hypotheses B1 (2.12) and B2 (2.14) below are stricter than the implicit conditions in [16] (more precisely these are derived from the trace-class assumption [16, Hypothesis 2.1], c.f. [16, Lemma 4.4]).

Hypothesis 2.12 (Hypothesis B1)**.** Assume that for all $\phi \in \mathrm{Dom}\,(A_-)$ and $\psi \in \mathrm{Dom}\left(A_-^2\right)$ we have $\langle \phi, A'(\cdot)\, \psi \rangle_{\mathrm{Dom}(A_-)_\Gamma} \in L^1(\mathbb{R})$ and

$$\begin{aligned}
&\int_{x_0}^{x} \langle \phi, A'(y)\, \psi \rangle_{\mathrm{Dom}(A_-)_\Gamma} \mathrm{d}y = \langle \phi, (A(x) - A(x_0))\, \psi \rangle_{\mathrm{Dom}(A_-)_\Gamma}, \quad x, x_0 \in \mathbb{R}, \\
&\lim_{x \to -\infty} \langle \phi, A(x)\, \psi \rangle_{\mathrm{Dom}(A_-)_\Gamma} = \langle \phi, A_- \psi \rangle_{\mathrm{Dom}(A_-)_\Gamma}, \\
&x \mapsto A(x)\, \phi \text{ is continuous.}
\end{aligned} \tag{52}$$

We also assume that

$$\operatorname*{ess\,sup}_{x\in\mathbb{R}}\left\|A'(x)\left(A_-^2+z\right)^{-1}\right\|_{B(H)}\xrightarrow{z\to+\infty}0. \tag{53}$$

Furthermore we assume that there exists $z>1$, such that

$$\sup_{x\in\mathbb{R}}\left\|\left(A(x)^2-A_-^2\right)\left(A_-^2+z\right)^{-1}\right\|_{B(H)}<1. \tag{54}$$

Remark 2.13. Note that condition (53) is satisfied if

$$\operatorname*{ess\,sup}_{x\in\mathbb{R}}\left\|A'(x)\left(A_-^2+1\right)^{-1/2}\right\|_{B(H)}<\infty, \tag{55}$$

or in other words, if $A'(x)$, $x\in\mathbb{R}$, is an essentially uniformly bounded family of bounded operators from $\operatorname{Dom}(A_-)_\Gamma$ to H.

As an alternative to Hypothesis B1 (2.12) we give a version, which is centred around a family of "scaling" operators $B(x)\,,\ x\in\mathbb{R}$. The purpose here is to mitigate the following issue with Hypothesis B1 (2.12), which does not occur in [16, Hypothesis 2.1].
Assume that we introduce a sufficiently regular, compactly supported scalar function $\rho(x)\,,\ x\in\mathbb{R}$. If we consider the commutative family $A(x)=\rho(x)A_-+A_-,\ x\in\mathbb{R}$, then the Hypotheses A1 (2.10), A2 (2.11) or [16, Hypothesis 2.1] can be satisfied for all choices of ρ, if A_- possesses an appropriate discrete spectrum. Also conditions (52) and (53) allow for such non-trivial choices, which can be easily verified. However, if A_- is unbounded, then condition (54) is equivalent to

$$\sup_{x\in\mathbb{R}}\left|\rho(x)^2+2\rho(x)\right|<1, \tag{56}$$

which is very restrictive and even shows that it fails to hold, if ρ is replaced by a multiple $\lambda\rho$ with a sufficiently large number λ (of course for $\rho\neq 0$.). This strange "non-scalability" of condition (54) is disturbing, if we consider the overall goal of finding a version of the "index=spectral flow"-theorem, where both sides of the equation are invariant under arbitrarily scaling the perturbation $A(x)-A_-$, $x\in\mathbb{R}$, by a constant.
We therefore introduce the slightly more complicated to formulate Hypothesis B2 (2.14), which, however, retains stability under the above demonstrated scaling.

Hypothesis 2.14 (Hypothesis B2)**.** We assume there is a strongly continuous family of bounded operators $(B(x))_{x\in\mathbb{R}}\subset B(H)\cap B\left(\operatorname{Dom}(A_-)_\Gamma\right)\cap B\left(\operatorname{Dom}\left(A_-^2\right)_\Gamma\right)$ and that there exists a bounded operator $B_0\in B(H)\cap B\left(\operatorname{Dom}(A_-)_\Gamma\right)\cap B\left(\operatorname{Dom}\left(A_-^2\right)_\Gamma\right)$, which is invertible in H, $\operatorname{Dom}(A_-)_\Gamma$ and in $\operatorname{Dom}\left(A_-^2\right)_\Gamma$.
We assume that

$$\sup_{x\in\mathbb{R}}\left\|A'(x)\left((B_0^*A_-B_0)^2+z\right)^{-1}\right\|_{B(H)}\xrightarrow{z\to+\infty}0. \tag{57}$$

Furthermore we assume that for

$$\begin{aligned} R_1(x) &:= A(x) - B(x)^* A_- B(x), \\ R_2(x) &:= A(x)^2 - \left(B(x)^* A_- B(x)\right)^2, \end{aligned} \tag{58}$$

there exist $C < \infty$, $0 < \epsilon < 1$, and $0 \leq \alpha < 1$ such that for $i \in \{1, 2\}$

$$\sup_{x\in\mathbb{R}} \left\| \left(\left(B(x)^* A_- B(x)\right)^i - \left(B_0^* A_- B_0\right)^i \right) \left(\left(B_0^* A_- B_0\right)^2 + 1 \right)^{-i/2} \right\|_{B(H)} \leq \epsilon, \tag{59}$$

$$\sup_{x\in\mathbb{R}} \left\| R_i(x) \left(\left(B_0^* A_- B_0\right)^2 + 1 \right)^{-i\alpha/2} \right\|_{B(H)} \leq C. \tag{60}$$

To give Hypothesis B2 (2.14) some perspective, motivated from the theory of pseudo-differential operators (c.f. [36]), we should think of $B(x)$, $x \in \mathbb{R}$, as a family of scaling operators, thus $B(x)^* A_- B(x)$, $x \in \mathbb{R}$, as the "leading operators" and of the operator families $R_i(x)$, $x \in \mathbb{R}$, as operators of "lower order" (condition (60)).

Let us now compare the central Hypotheses A1 (2.10) and A2 (2.11) to the condition

$$\int_{\mathbb{R}} \left\| A'(x) \left(A_-^2 + 1\right)^{-1/2} \right\|_{S^1(H)} \mathrm{d}x < \infty, \tag{61}$$

which is the central condition of [16, Hypothesis 2.1].

Lemma 2.15. *Assume [16, Hypothesis 2.1] (in particular condition (*61*)). Then also Hypothesis A2 (*2.11*) and thus Hypothesis A1 (*2.10*) hold. More precisely, [16, Hypothesis 2.1] implies that for $t, s > 0$ the operator,*

$$e^{-tA_-^2} A'(x) e^{-sA_-^2},$$

is trace-class in H, the function

$$y \mapsto \left\| e^{-tA_-^2} A'(y) e^{-sA_-^2} \right\|_{S^1(H)},$$

is integrable over $\mathbb{R}$ and we obtain for all $\epsilon > 0$,

$$\left((u, v) \mapsto \int_{\mathbb{R}} \left\| e^{-uA_-^2} A'(y) e^{-vA_-^2} \right\|_{S^1(H)} \mathrm{d}y \right) \in I^{log}_{-1+\epsilon,-1/2+\epsilon} \cap I^{log}_{-1/2+\epsilon,-1+\epsilon}. \tag{62}$$

Proof. For $t, s > 0$ we may write

$$e^{-tA_-^2} A'(x) e^{-sA_-^2} = e^{-tA_-^2} \left(A'(x) \left(A_-^2 + 1\right)^{-1/2} \right) \left(\left(A_-^2 + 1\right)^{+1/2} e^{-sA_-^2} \right), \tag{63}$$

which immediately shows that $e^{-tA_-^2} A'(x) e^{-sA_-^2}$ is trace-class in H and that

$$y \mapsto \left\| e^{-tA_-^2} A'(y) e^{-sA_-^2} \right\|_{S^1(H)}$$

is integrable over $\mathbb{R}$ by [16, Hypothesis 2.1]. On the other hand, if an operator T is trace class in H, then also T^* is trace-class in H, with the same trace norm[6]. Therefore, we estimate for $t_0 > 0$, by Corollary 2.39,

$$\begin{aligned}
&\int_0^{t_0}\int_0^{t_0}\int_{\mathbb{R}} \log(t)\log(s)\, t^{-1+\epsilon} s^{-1/2+\epsilon} \left\| e^{-tA_-^2} A'(x)\, e^{-sA_-^2} \right\|_{S^1(H)} \mathrm{d}x\ \mathrm{d}t\ \mathrm{d}s \\
\leq &\int_0^{t_0}\int_0^{t_0} \log(t)\log(s)\, t^{-1+\epsilon} s^{-1/2+\epsilon} \\
&\qquad \int_{\mathbb{R}} \left\| A'(x)\left(A_-^2+1\right)^{-1/2} \right\|_{S^1(H)} \left\| \left(A_-^2+1\right)^{1/2} e^{-sA_-^2} \right\|_{B(H)} \mathrm{d}x\ \mathrm{d}t\ \mathrm{d}s \\
\lesssim_{t_0} &\int_{\mathbb{R}} \left\| A'(x)\left(A_-^2+1\right)^{-1/2} \right\|_{S^1(H)} \mathrm{d}x \cdot \int_0^{t_0}\int_0^{t_0} \log(t)\log(s)\, t^{-1+\epsilon} s^{-1+\epsilon} \mathrm{d}t\ \mathrm{d}s \\
< &\infty. \\
&\int_0^{t_0}\int_0^{t_0}\int_{\mathbb{R}} \log(t)\log(s)\, t^{-1/2+\epsilon} s^{-1+\epsilon} \left\| e^{-tA_-^2} A'(x)\, e^{-sA_-^2} \right\|_{S^1(H)} \mathrm{d}x\ \mathrm{d}t\ \mathrm{d}s \\
\leq &\int_0^{t_0}\int_0^{t_0} \log(t)\log(s)\, t^{-1/2+\epsilon} s^{-1+\epsilon} \left\| \left(A_-^2+1\right)^{1/2} e^{-tA_-^2} \right\|_{B(H)} \\
&\qquad \int_{\mathbb{R}} \left\| \left\{ \left(A_-^2+1\right)^{-1/2} A'(x) \right\} \right\|_{S^1(H)} \mathrm{d}x\ \mathrm{d}t\ \mathrm{d}s \\
\lesssim_{t_0} &\int_{\mathbb{R}} \left\| A'(x)\left(A_-^2+1\right)^{-1/2} \right\|_{S^1(H)} \mathrm{d}x \cdot \int_0^{t_0}\int_0^{t_0} \log(t)\log(s)\, t^{-1+\epsilon} s^{-1+\epsilon} \mathrm{d}t\ \mathrm{d}s \\
< &\infty.
\end{aligned} \tag{64}$$

Thus we conclude that

$$\left((u,v) \mapsto \int_{\mathbb{R}} \left\| e^{-uA_-^2} A'(y)\, e^{-vA_-^2} \right\|_{S^1(H)} \mathrm{d}y \right) \in I^{log}_{-1+\epsilon,-1/2+\epsilon} \cap I^{log}_{-1/2+\epsilon,-1+\epsilon}, \tag{65}$$

which implies Hypothesis A2 (2.10) and A1 (2.10). ■

Remark 2.16. In view of the estimates in (64), we note that Hypothesis A2 (2.11) is still satisfied if we replace condition (61) in [16, Hypothesis 2.1] by (the weaker requirement)

$$\begin{aligned}
&\int_{\mathbb{R}} \left\| \left(1+A_-^2\right)^{-1/4+\epsilon} A'(x) \left(1+A_-^2\right)^{-3/4+\epsilon} \right\|_{S^1(H)} \mathrm{d}x < \infty, \\
&\int_{\mathbb{R}} \left\| \left(1+A_-^2\right)^{-3/4+\epsilon} A'(x) \left(1+A_-^2\right)^{-1/4+\epsilon} \right\|_{S^1(H)} \mathrm{d}x < \infty,
\end{aligned} \tag{66}$$

for some $\epsilon > 0$.

[6] Since $T = S_1 S_2$ splits into two Hilbert-Schmidt operators in H with $\|S_1\|_{S^2(H)} = \|S_2\|_{S^2(H)} = \|T\|^{1/2}_{S^1(H)}$, we conclude that $T^* = S_2^* S_1^*$ is the product of two Hilbert-Schmidt operators, because the Schwartz kernels of S_i^* are $(x,y) \mapsto \overline{k_i(y,x)}$, if k_i are the Schwartz kernels of S_i, for $i = 1,2$. The Hilbert-Schmidt norms of S_1^* and S_2^* are the same as those of S_1, and S_2 respectively. Thus T^* is trace-class with trace-norm $\|T^*\|_{S^1(H)} \leq \|T\|_{S^1(H)}$. If we apply the adjoint again, we achieve equality of the trace-norms.

To illustrate the last Remark, let us duplicate [16, Example 3.15] and amend it, such that Hypothesis A2 (2.11) is satisfied. Note that versions of the cited example and the example below have been discussed in [37] and originated from [7].

Example 2.17. Let $n, k \in \mathbb{N}$, $k > p > \frac{2}{3}n$, $q > n/2$ and $\epsilon > 0$. Consider

$$\begin{aligned}
0 \leq V_- &\in L^2\left(\mathbb{R}^n, \left(1+|\xi|^2\right)^q \mathrm{d}^n\xi\right) \cap L^\infty\left(\mathbb{R}^n, \mathrm{d}^n\xi\right), \\
0 \leq V(x,\cdot) &\in L^2\left(\mathbb{R}^n, \left(1+|\xi|^2\right)^q \mathrm{d}^n\xi\right) \cap L^\infty\left(\mathbb{R}^n, \mathrm{d}^n\xi\right), \\
\partial_x V(x,\cdot) &\in L^2\left(\mathbb{R}^n, \left(1+|\xi|^2\right)^q \mathrm{d}^n\xi\right) \cap L^\infty\left(\mathbb{R}^n, \mathrm{d}^n\xi\right), \\
\mathbb{R} \ni x \mapsto \partial_x V(x,\cdot) &\in C^k\left(\mathbb{R}, L^\infty\left(\mathbb{R}^n, \mathrm{d}^n\xi\right)\right), \\
\int_{\mathbb{R}} \|\partial_x V(x,\cdot)\|_{L^2\left(\mathbb{R}^n, \left(1+|\xi|^2\right)^q \mathrm{d}^n\xi\right)} \mathrm{d}x &< \infty.
\end{aligned} \tag{67}$$

If we denote the operator of multiplication by V_-, V, and $\partial_x V$ in $L^2(\mathbb{R}^n, \mathrm{d}^n x)$ by the same letter, we may introduce

$$\begin{aligned}
A_- &:= (-\Delta)^{p/2} + V_- + \epsilon,\ \mathrm{Dom}(A_-) = \mathrm{Dom}\left((-\Delta)^{p/2}\right) = W^{p,2}(\mathbb{R}^n), \\
A(x) &:= A_- + V(x,\cdot) - V_-,\ \mathrm{Dom}(A(x)) = \mathrm{Dom}(A_-) = W^{p,2}(\mathbb{R}^n),
\end{aligned} \tag{68}$$

where $-\Delta$ is the self-adjoint Laplacian in $L^2(\mathbb{R}^n, \mathrm{d}^n\xi)$, with domain $W^{2,2}(\mathbb{R}^n)$, $W^{k,2}(\mathbb{R}^n)$ denoting the L^2-Sobolev spaces of order k. The domain properties are easily checked, because $V(x,\cdot)$, $x \in \mathbb{R}$ and V_- are $L^\infty(\mathbb{R}^n)$-elements, thus constituting bounded multiplication operators in $L^2(\mathbb{R}^n)$. Since $p > \frac{2}{3}n$ and $q > n/2$ we have for some $\delta > 0$ small enough

$$\xi \mapsto \left(|\xi|^2 + 1\right)^{-\frac{3}{4}p+\delta} \in L^2\left(\mathbb{R}^n, \left(1+|\xi|^2\right)^q \mathrm{d}^n\xi\right), \tag{69}$$

and thus, applying [37, Corollary 4.8], we obtain for $\delta > 0$ small enough,

$$[\partial_x V(x,\cdot)]\left((-\Delta)^p + 1\right)^{-3/4+\delta} \in S^1\left(L^2\left(\mathbb{R}^n, \mathrm{d}^n\xi\right)\right),\ x \in \mathbb{R}, \tag{70}$$

which implies for $\delta > 0$ small enough,

$$A'(x)\left(A_-^2 + 1\right)^{-3/4+\delta} \in S^1(H),\ x \in \mathbb{R}, \tag{71}$$

with $H = L^2(\mathbb{R}^n, \mathrm{d}^n\xi)$. Thus, in consideration of Remark 2.16, we conclude that Hypothesis A2 (2.11) holds for this family of operators $A(x)$, $x \in \mathbb{R}$.
Note also that the C^k-regularity and L^∞-conditions in (67) imply that, on the one hand Hypothesis B2 (2.14), with the trivial choice $B_0 = B(x) = 1$, $x \in \mathbb{R}$, holds for the family $A(x)$, $x \in \mathbb{R}$, while on the other hand also the remaining conditions from Definition 2.3 are satisfied.

Example 2.17 shows that we are able to decrease the power of the Laplacian power from $p > n$ in [16, Example 3.15] to $p > \frac{2}{3}n$ here, while we have to increase the regularity of V from C^1 in [16, Example 3.15] to C^k, $k > n$, to cope with our domain requirements.

With this example illustrating the trade-off between [16] and our work, we close the discussion of the Hypotheses. Before we proceed to present the consequences of the hypotheses, let us review a selection of classical operator norm inequalities, which we will use in abundance.

2.3 Some operator norm inequalities

Operator norm inequalities are a field in its own right with many well-known results (for example, and taking a central role, the famous Heinz and Heinz-Kato inequalities (c.f. [19],[21])). This subsection is dedicated to review some of those inequalities, which have been used in some related form also in [16, Theorem 4.1] and [26], and are also of some relevance to theory of Hilbert scales (c.f. [9]). However, since we will use some of them regularly we will prove them here in a self-contained manner.

Let T be an (unbounded,) positive operator in a Hilbert space H and let S be densely defined, and closable in H. It should be noted that in this situation, we have always the following implications:

$$\begin{aligned} &\mathrm{Dom}\left(\overline{S}\right) \supseteq \mathrm{Dom}\left(T\right), \ ST^{-1} \text{ is densely defined,} \\ \Longleftrightarrow &\mathrm{Dom}\left(\overline{S}\right)_\Gamma \supseteq \mathrm{Dom}\left(T\right)_\Gamma, \ ST^{-1} \text{ is densely defined,} \\ \Longleftrightarrow &\left\{\overline{S}T^{-1}\right\} = \left\{ST^{-1}\right\} \text{ exist.} \end{aligned} \tag{72}$$

$$\mathrm{Dom}\left(S\right) \supseteq \mathrm{Dom}\left(T\right) \Longrightarrow \left\{\overline{S}T^{-1}\right\} = \left\{ST^{-1}\right\} \text{ exist.} \tag{73}$$

The first equivalence of the first line is due to the closed graph theorem. For the implication of the second line one uses the first line. In both lines one uses that ST^{-1} is closable and $\overline{ST^{-1}} = \overline{S}T^{-1}$.

Let us present an important consequence of the method of complex interpolation for operator norms.

Lemma 2.18. *If* $\left\{T^{-1}S\right\}$ *and* $\left\{ST^{-1}\right\}$ *exist, then so does* $\left\{T^{-x}\overline{S}T^{-1+x}\right\}$*, for all* $x \in [0,1]$*. Furthermore*

$$\left\|\left\{T^{-x}\overline{S}T^{-1+x}\right\}\right\|_{B(H)} \leq \left\|\left\{ST^{-1}\right\}\right\|_{B(H)}^{1-x} \cdot \left\|\left\{T^{-1}S\right\}\right\|_{B(H)}^{x}, \ x \in [0,1]. \tag{74}$$

If additionally $\mathrm{Dom}\left(S\right) \supseteq \mathrm{Dom}\left(T\right)$*, then also* $\left\{T^{-x}ST^{-1+x}\right\}$*,* $x \in [0,1]$*, exists and* $\left\{T^{-x}ST^{-1+x}\right\} = \left\{T^{-x}\overline{S}T^{-1+x}\right\}$*,* $x \in [0,1]$*.*

Proof. We first show that for $x \in [0,1]$, the operator $T^{-x}ST^{-1+x}$ is closable. Let $\phi_n \in \mathrm{Dom}\left(T^{-x}ST^{-1+x}\right)$ be a sequence such that $\phi_n \to 0$ in H and $T^{-x}ST^{-1+x}\phi_n \to \psi$ in H. Let $C = T^{-1}S$. Then $T^{-x}ST^{-1+x}\phi_n = T^{1-x}CT^{-1+x}\phi_n$. Since the operator T^{1-x} has a bounded inverse, we conclude

$$CT^{-1+x}\phi_n \to T^{-1+x}\psi \text{ in } H. \tag{75}$$

Since T^{-1+x} is bounded we have that $T^{-1+x}\phi_n \to 0$ in H. Because C is closable and $T^{-1+x}\phi_n \in \mathrm{Dom}\,(C)$ we conclude that $T^{-1+x}\psi = 0$ and thus $\psi = 0$. Therefore $T^{-x}ST^{-1+x}$ is closable.
Let $\phi \in H$ and $\psi \in \mathrm{Dom}\,(T) \subseteq \mathrm{Dom}\,(\overline{S})$ and define

$$f_{\phi,\psi}\,(z) := \langle \phi, T^{-z}\overline{S}T^{-1+z}\psi \rangle_H. \tag{76}$$

The function f is holomorphic on $\{z \in \mathbb{C},\ 0 < \Re z < 1\}$. Define

$$M_{\phi,\psi}\,(x) := \sup_{y\in\mathbb{R}} |f\,(x+iy)|\,, \tag{77}$$

the supremum on each vertical line through x. Therefore, by Hadamard's Three-lines Theorem (c.f. [32, p.33-34]), we have

$$M_{\phi,\psi}\,(x) \le M_{\phi,\psi}\,(0)^{1-x}\, M_{\phi,\psi}\,(1)^{x}\,. \tag{78}$$

Furthermore we have that

$$T^{-x}\overline{S}T^{-1+x}\mathbb{1}_{[0,n]}\,(T)\,\psi \xrightarrow{n\to\infty} T^{-x}\overline{S}T^{-1+x}\psi, \tag{79}$$

since $\psi \in \mathrm{Dom}\,(T)$. But then, by inequality (78), we have for all $n \in \mathbb{N}$ and by putting

$$X := \{\phi \in H, \psi \in \mathrm{Dom}\,(T)\,|\,\|\phi\| = \|\psi\| = 1\}\,, \tag{80}$$

the inequality

$$\begin{aligned}\left\|T^{-x}\overline{S}T^{-1+x}\mathbb{1}_{[0,n]}\,(T)\right\|_{B(H)} &\le \sup_{\substack{\psi\in\mathrm{Dom}(T),\|\psi\|=1\\ y\in\mathbb{R}}} \left\|T^{-x-iy}\overline{S}T^{-1+x+iy}\psi\right\|_H = \sup_{(\phi,\psi)\in X} M_{\phi,\psi}\,(x)\\ &\le \sup_{(\phi,\psi)\in X} M_{\phi,\psi}\,(0)^{1-x} \cdot \sup_{(\phi,\psi)\in X} M_{\phi,\psi}\,(1)^{x}\\ &\le \left\|\left\{ST^{-1}\right\}\right\|_{B(H)}^{1-x} \cdot \left\|\left\{T^{-1}S\right\}\right\|_{B(H)}^{x}\,. \end{aligned} \tag{81}$$

Since $\mathrm{Dom}\,(T)$ is dense, we conclude, by the uniform boundedness principle, that $T^{-x}\overline{S}T^{-1+x}\mathbb{1}_{[0,n]}\,(T)$ must converge strongly on H to some linear bounded operator B in H. On the other hand, for $\psi \in H$, we see that

$$\psi_n := \mathbb{1}_{[0,n]}\,(T)\,\psi \in \mathrm{Dom}\,(T) \subseteq \mathrm{Dom}\left(T^{-x}\overline{S}T^{-1+x}\right), \tag{82}$$

and $\psi_n \to \psi$ in H. Furthermore, $T^{-x}\overline{S}T^{-1+x}\psi_n \xrightarrow{n\to\infty} B\psi$ in H. Since $T^{-x}\overline{S}T^{-1+x}$ is closable, we conclude that $\psi \in \mathrm{Dom}\left(\overline{T^{-x}\overline{S}T^{-1+x}}\right)$ and $B = \overline{T^{-x}\overline{S}T^{-1+x}}$. So $\left\{T^{-x}\overline{S}T^{-1+x}\right\}$ exists and we can estimate the operator norm, according to the inequality (81),

$$\left\|\left\{T^{-x}\overline{S}T^{-1+x}\right\}\right\|_{B(H)} = \|B\|_{B(H)} \le \left\|\left\{ST^{-1}\right\}\right\|^{1-x} \cdot \left\|\left\{T^{-1}S\right\}\right\|_{B(H)}^{x}. \tag{83}$$

In the case that $\mathrm{Dom}\,(S) \supseteq \mathrm{Dom}\,(T)$, we can copy the proof ad verbatim, starting with the construction of $f_{\phi,\psi}\,(z)$, and ending with the last line by replacing $\overline{S}$ with S everywhere.

Therefore both $\{T^{-x}ST^{-1+x}\}$ and $\{T^{-x}\overline{S}T^{-1+x}\}$ exist. Clearly both are bounded operators in H, which coincide on the dense subset $\mathrm{Dom}\,(T)$ of H (Because they are closures of operators already coinciding on $\mathrm{Dom}\,(T)$). Therefore

$$\left\{T^{-x}ST^{-1+x}\right\} = \left\{T^{-x}\overline{S}T^{-1+x}\right\}. \tag{84}$$

■

The above interpolation lemma raises the question in which cases $\{T^{-1}S\}$ exists.

Lemma 2.19. *Let B be a bounded operator in H. Assume $\{S^*B^*\}$ exists, then also $\{BS\}$ exists, and*

$$\|\{BS\}\|_{B(H)} \leq \|\{S^*B^*\}\|_{B(H)}. \tag{85}$$

Proof. Since S is densely defined, S^* exists and we have

$$(BS)^* = S^*B^*, \tag{86}$$

which is an everywhere defined operator, in particular the adjoint of BS is densely defined and therefore BS is closable.
On $\mathrm{Dom}\left(\overline{S}\right)$ we may write, using the right side polar decomposition of $\overline{S}$,

$$\begin{aligned} B\overline{S} &= BCP, \\ C &:= |S^*| = \left(\overline{S}S^*\right)^{1/2}, \end{aligned} \tag{87}$$

for an appropriate partial isometry P. Let $C_n := \mathbb{1}_{[-n,n]}(C)$. Then BC_nP converges strongly on $\mathrm{Dom}\,(S)$ to BS. On the other hand,

$$\|BC_nP\|_{B(H)} \leq \|BC_n\|_{B(H)} = \|C_nB^*\|_{B(H)}. \tag{88}$$

Here, we used the self-adjointness of C_n. Since CB^* is a bounded operator, because $\mathrm{Dom}\,(C)_\Gamma = \mathrm{Dom}\,(S^*)_\Gamma$ and $\{S^*B^*\}$ exists, the terms of (88) must be uniformly bounded in n by $\|\{CB^*\}\|_{B(H)}$. Hence, by the uniform boundedness principle, BC_nP converges strongly to a bounded operator A in H. Since taking adjoints is continuous with respect to the weak operator topology, we have for $\phi, \psi \in H$,

$$\langle \phi, S^*B^*\psi\rangle_H \xleftarrow{n\to\infty} \langle \phi, P^*C_nB^*\psi\rangle_H \xrightarrow{n\to\infty} \langle \phi, A^*\psi\rangle_H, \tag{89}$$

and thus $A^* = S^*B^*$. By equality (86) we therefore find

$$A = A^{**} = (S^*B^*)^* = (BS)^{**} = \overline{BS}, \tag{90}$$

so $\{BS\}$ exists. Finally we have by the remark following (88),

$$\|\{BS\}\|_{B(H)} \leq \|\{CB^*\}\|_{B(H)} = \|\{S^*B^*\}\|_{B(H)}. \tag{91}$$

■

Remark 2.20. Especially, if S is symmetric and $\mathrm{Dom}(S) \supseteq \mathrm{Dom}(T)$, the prerequisites of Lemma 2.19 are satisfied. Therefore both $\{T^{-1}S\}$ and $\{ST^{-1}\}$ exist, and we may conclude by Lemma 2.18, that also $\{T^{-x}ST^{-1+x}\}$ exists for $x \in [0,1]$, and,

$$\left\|\left\{T^{-x}ST^{-1+x}\right\}\right\|_{B(H)} \leq \left\|ST^{-1}\right\|_{B(H)}, \ x \in [0,1]. \tag{92}$$

Finally, we present the following norm inequality, involving the powers of both S and T^{-1}, and is sometimes referred to as the Cordes' inequality.

Lemma 2.21. *Let S be additionally non-negative and self-adjoint and assume $\{ST^{-1}\}$ exists. Then, for $x \in [0,1]$, also $\{S^x T^{-x}\}$ exists, and*

$$\left\|\left\{S^x T^{-x}\right\}\right\|_{B(H)} \leq \left\|\left\{ST^{-1}\right\}\right\|_{B(H)}^x. \tag{93}$$

Proof. We begin by noting that $S^x T^{-x}$ is closed, since S^x is closed and T^{-x} is bounded. The rest of the proof is similar to the proof of Lemma 2.18, so we will only give an outline. For $\phi \in H$ and $\psi \in \mathrm{Dom}(T)$ we define

$$g_{\phi,\psi}(z) := \langle \phi, S^z T^{-z} \psi \rangle_H, \tag{94}$$

which is holomorphic on $\{z \in \mathbb{C}, \ 0 < \Re z < 1\}$. Taking suprema on vertical lines and over ϕ and ψ appropriately, we arrive at the estimate

$$\left\|S^x T^{-x} \mathbb{1}_{[0,n]}(T)\right\|_{B(H)} \leq 1 \cdot \left\|\left\{ST^{-1}\right\}\right\|_{B(H)}^x, \tag{95}$$

using Hadamard's three-lines theorem. The uniform boundedness principle allows us to conclude that the above estimated sequence of bounded operators must converge to a bounded operator, satisfying the same estimate in norm. This limit, however, must also be the closure of $S^x T^{-x}$. ■

An obvious first use of the above norm inequality is to apply it to the family $A(x)$, $x \in \mathbb{R}$, and its properties in Definition 2.3.

Corollary 2.22. $\mathrm{Dom}(A(x)) = \mathrm{Dom}(A_-), \ x \in \mathbb{R}$.

Proof. Since we have equality of domains $\mathrm{Dom}\left(A(x)^2\right) = \mathrm{Dom}\left(A_-^2\right)$, $x \in \mathbb{R}$, we conclude that

$$\left\{\left(1 + A(x)^2\right)\left(1 + A_-^2\right)^{-1}\right\}, \ x \in \mathbb{R},$$

exists. By Lemma 2.21 we conclude that also

$$\left\{\left(1 + A(x)^2\right)^{1/2}\left(1 + A_-^2\right)^{-1/2}\right\}, \ x \in \mathbb{R},$$

exists. Because

$$\mathrm{Dom}(A_-) = \mathrm{Dom}\left(\left(1 + A_-^2\right)^{1/2}\right), \ \mathrm{Dom}(A(x)) = \mathrm{Dom}\left(\left(1 + A(x)^2\right)^{1/2}\right), \ x \in \mathbb{R}, \tag{96}$$

by the functional calculus of the involved operators, the inclusion $\mathrm{Dom}(A(x)) \supseteq \mathrm{Dom}(A_-)$ must hold. By interchanging the roles of A_- and $A(x)$, $x \in \mathbb{R}$, we also have the reverse inclusion $\mathrm{Dom}(A(x)) \subseteq \mathrm{Dom}(A_-)$, $x \in \mathbb{R}$. ■

In the next subsection we will discuss the first consequences of the Hypotheses B1 (2.12) or B2 (2.14) for the family $A(x)$, $x \in \mathbb{R}$, and we will make some further use of the norm inequalities in this subsection.

2.4 Basic properties and further definitions

The goal of this subsection is to introduce the operators A_+ in H, D, and $H_\pm$ in $L^2(\mathbb{R}, H)$, which are the basic objects of inquiry of this work. We do so by applying the Kato-Rellich estimates from Hypothesis B1 (2.12) or Hypothesis B2 (2.14) to the (unperturbed) operators D_0 and H_0. We therefore follow the approach in [16] closely, however with the necessary amendments. We close the subsection by giving a version of Duhamel's formula, and we introduce several operators comprised of D and $H_\pm$, which play a key role in calculating the trace formula later on.

We begin by discussing a uniform norm bound on the family $A(x)$, $x \in \mathbb{R}$.

Lemma 2.23. $\sup_{x\in\mathbb{R}} \|A(x)\|_{B\left(\mathrm{Dom}(A_-)_\Gamma, H\right)} + \sup_{x\in\mathbb{R}} \|A(x)\|_{B\left(\mathrm{Dom}\left(A_-^2\right)_\Gamma, \mathrm{Dom}(A_-)_\Gamma\right)} < \infty$.

Proof. For $\phi \in H$ and $\psi \in \mathrm{Dom}(A_-)$, we know that $(y \mapsto \langle \phi, A'(y)\psi\rangle_H) \in L^1(\mathbb{R})$, by Definition 2.3. Therefore,

$$\sup_{x\in\mathbb{R}} |\langle \phi, (A(x) - A_-)\psi\rangle_H| \leq \int_{\mathbb{R}} \left|\langle \phi, A'(y)\psi\rangle_H\right| \mathrm{d}y < \infty, \tag{97}$$

and thus, by the uniform boundedness principle applied to $\phi \in H$ and $\psi \in \mathrm{Dom}(A_-)$, we obtain

$$\sup_{x\in\mathbb{R}} \|A(x) - A_-\|_{B\left(\mathrm{Dom}(A_-)_\Gamma, H\right)} < \infty, \tag{98}$$

which shows, since A_- is a constant operator in $B(\mathrm{Dom}(A_-)_\Gamma, H)$, that

$$\sup_{x\in\mathbb{R}} \|A(x)\|_{B\left(\mathrm{Dom}(A_-)_\Gamma, H\right)} < \infty. \tag{99}$$

The inequality

$$\sup_{x\in\mathbb{R}} \|A(x)\|_{B\left(\mathrm{Dom}\left(A_-^2\right)_\Gamma, \mathrm{Dom}(A_-)_\Gamma\right)} < \infty, \tag{100}$$

is shown analogously. ■

Let us show that the chosen Hypotheses B1 (2.12) or B2 (2.14) and Definition 2.3 already suffice to determine the limit of the family $A(x)$, $x \in \mathbb{R}$, at $+\infty$. This limiting operator A_+ retains some of the properties A_- possesses, the limit of $A(x)$, $x \in \mathbb{R}$ at $-\infty$, underlining the symmetry of our setup.

Lemma 2.24. *Assume one of the Hypotheses B1 (*2.12*) or B2 (*2.14*). Then there exists a self-adjoint operator A_+ in H with domain* $\mathrm{Dom}(A_+) = \mathrm{Dom}(A_-)$*, such that for $\phi \in H$ and $\psi \in \mathrm{Dom}(A_-)$, we have*

$$\langle \phi, (A_+ - A_-)\psi\rangle_H = \int_{\mathbb{R}} \langle \phi, A'(y)\psi\rangle_H \mathrm{d}y. \tag{101}$$

Furthermore, we have $\mathrm{Dom}(A_+)_\Gamma = \mathrm{Dom}(A_-)_\Gamma$ *and* $\mathrm{Dom}\left(A_+^2\right)_\Gamma = \mathrm{Dom}\left(A_-^2\right)_\Gamma$.

Proof. We start by defining the operator A_+ with $\mathrm{Dom}(A_+) := \mathrm{Dom}(A_-)$ by equation (101). Apart from the apparent linearity of A_+, we may also conclude that A_+ is symmetric. However, the self-adjointness of A_+ requires the Hypotheses B1 (2.12) or B2 (2.14). Let us first assume Hypothesis B1 (2.12). Additional to equation (101), the operator A_+ must also fulfil the following equation for $\phi \in \mathrm{Dom}(A_-)$ and $\psi \in \mathrm{Dom}\left(A_-^2\right)$:

$$\langle \phi, (A_+ - A_-)\,\psi\rangle_{\mathrm{Dom}(A_-)_\Gamma} = \int_{\mathbb{R}} \langle \phi, A'(y)\,\psi\rangle_{\mathrm{Dom}(A_-)_\Gamma} \mathrm{d}y. \tag{102}$$

This implies that A_+ maps $\mathrm{Dom}\left(A_-^2\right)$ into $\mathrm{Dom}(A_-)$. Analogous to Lemma 2.23 we may conclude, by the uniform boundedness principle, and by denoting $A(+\infty) := A_+$, that

$$\begin{aligned} \sup_{x\in\mathbb{R}\cup\{+\infty\}} \|A(x)\|_{B\left(\mathrm{Dom}\left(A_-^2\right)_\Gamma, \mathrm{Dom}(A_-)_\Gamma\right)} &< \infty, \\ \sup_{x\in\mathbb{R}\cup\{+\infty\}} \|A(x)\|_{B\left(\mathrm{Dom}(A_-)_\Gamma, H\right)} &< \infty, \end{aligned} \tag{103}$$

The symmetric operator A_+^2 is thus densely defined on $\mathrm{Dom}\left(A_-^2\right)$, and we obtain for $\phi \in H$ and $\psi \in \mathrm{Dom}\left(A_-^2\right)$,

$$\begin{aligned} \langle \phi, \left(A_+^2 - A_-^2\right)\psi\rangle_H &= \int_{\mathbb{R}} \langle \phi, \big(A(y)\,A'(y) + A'(y)\,A(y)\big)\,\psi\rangle_H \mathrm{d}y \\ &= \lim_{x\to+\infty} \int_{-\infty}^{x} \langle \phi, \big(A(y)\,A'(y) + A'(y)\,A(y)\big)\,\psi\rangle_H \mathrm{d}y \\ &= \lim_{x\to+\infty} \langle \phi, \left(A(x)^2 - A_-^2\right)\psi\rangle_H. \end{aligned} \tag{104}$$

The first and third equality can be shown by assuming $\phi \in \mathrm{Dom}(A_-)$ first, considering the terms $\langle A_+\phi, A_+\psi\rangle_H$ and $\langle A(x)\,\phi, A(x)\,\psi\rangle_H$, pushing all operators in the integral representation to the side of ψ, and then extending the equation by density for all $\phi \in H$. Equation (104) also shows that for $z > 1$ large enough, we have

$$\left\|\left(A_+^2 - A_-^2\right)\left(A_-^2 + z\right)^{-1}\right\|_{B(H)} \leq \sup_{x\in\mathbb{R}} \left\|\left(A(x)^2 - A_-^2\right)\left(A_-^2 + z\right)^{-1}\right\|_{B(H)} < 1. \tag{105}$$

For $z > 1$ large enough we thus have the norm convergent (Neumann-) series in $B(H)$,

$$R := \left(A_-^2 + z\right)^{-1} \sum_{k=0}^{\infty} \left(-\left(A_+^2 - A_-^2\right)\left(A_-^2 + z\right)^{-1}\right)^k. \tag{106}$$

Clearly R also maps H into $\mathrm{Dom}\left(A_-^2\right)$. We check that R is a right and left inverse of the (densely defined, symmetric) operator $A_+^2 + z\big|_{\mathrm{Dom}\left(A_-^2\right)}$ and we conclude that $\mathrm{Dom}\left(A_-^2\right) \subseteq \mathrm{Dom}\left(A_+^2\right)$ is mapped by $A_+^2 + z$ onto H, and therefore that $A_+^2 + z$ must be already surjective. By a theorem of von Neumann on the deficiency indices, we conclude that A_+ is self-adjoint.
The estimate (105) also shows that $A_+^2 - A_-^2$ is relatively bounded by A_-^2 with Kato-Rellich

bound less than 1 (c.f. [22, Theorem V.4.3]), thus implying that $\mathrm{Dom}\left(A_-^2\right) = \mathrm{Dom}\left(A_+^2\right)$. The self-adjointness of A_+ and A_- then imply that the corresponding graph norms must be equivalent, and thus $\mathrm{Dom}\left(A_+^2\right)_\Gamma = \mathrm{Dom}\left(A_-^2\right)_\Gamma$. Lemma 2.21 finally implies $\mathrm{Dom}\left(A_+\right)_\Gamma = \mathrm{Dom}\left(A_-\right)_\Gamma$.

Let us now assume Hypothesis B2 (2.14) instead. For $z > 1$ we estimate, using the fact that A_+ is the weak operator limit on $\mathrm{Dom}\left(A_-\right)$ of $A(x)$ for $x \to +\infty$,

$$\begin{aligned}
&\left\| \left(A_+ - B_0^* A_- B_0\right)\left(\left(B_0^* A_- B_0\right)^2 + z\right)^{-1/2} \right\|_{B(H)} \\
\leq &\sup_{x\in\mathbb{R}} \left\| \left(A(x) - B_0^* A_- B_0\right)\left(\left(B_0^* A_- B_0\right)^2 + z\right)^{-1/2} \right\|_{B(H)} \\
\leq &\epsilon + C \cdot \left\| \left(\left(B_0^* A_- B_0\right)^2 + z\right)^{\alpha/2}\left(\left(B_0^* A_- B_0\right)^2 + z\right)^{-1/2} \right\|_{B(H)} \\
\leq &\epsilon + C \cdot z^{-1/2+\alpha/2}. \qquad (107)
\end{aligned}$$

We note that since $\epsilon < 1$ and $\alpha < 1$, we may choose z large enough such that the estimate is strictly smaller than 1. This implies that there is a constant $C' < \infty$ and $\epsilon' < 1$ such that for $\phi \in \mathrm{Dom}\left(B_0^* A_- B_0\right) = \mathrm{Dom}\left(A_-\right)$, we have the Kato-Rellich estimate

$$\left\| \left(A_+ - B_0^* A_- B_0\right)\phi \right\|_H \leq \epsilon' \left\| B_0^* A_- B_0 \phi \right\|_H + C' \left\|\phi\right\|_H. \qquad (108)$$

Therefore $A_+ = A_+ - B_0^* A_- B_0 + B_0^* A_- B_0$ is self-adjoint on the domain of $\mathrm{Dom}\left(B_0^* A_- B_0\right) = \mathrm{Dom}\left(A_-\right)$ by Kato-Rellich's theorem (c.f. [22, Theorem V.4.3]) and thus $\mathrm{Dom}\left(A_+\right)_\Gamma = \mathrm{Dom}\left(A_-\right)_\Gamma$.

Similarly one obtains

$$\begin{aligned}
&\left\| \left(A_+^2 - \left(B_0^* A_- B_0\right)^2\right)\left(\left(B_0^* A_- B_0\right)^2 + z\right)^{-1} \right\|_{B(H)} \\
\leq &\epsilon + C \cdot z^{-1+\alpha}, \qquad (109)
\end{aligned}$$

which shows that $A_+^2 = A_+^2 - \left(B_0^* A_- B_0\right)^2 + \left(B_0^* A_- B_0\right)^2$ is self-adjoint on the domain of $\mathrm{Dom}\left(\left(B_0^* A_- B_0\right)^2\right) = \mathrm{Dom}\left(A_-^2\right)$ by Kato-Rellich's theorem (c.f. [22, Theorem V.4.3]), and therefore $\mathrm{Dom}\left(A_+^2\right)_\Gamma = \mathrm{Dom}\left(A_-^2\right)_\Gamma$. ■

Let us now introduce the operator D in $L^2(\mathbb{R}, H)$, which is the focal point of our investigation in $L^2(\mathbb{R}, H)$.

Definition 2.25.

$$D := \partial + A(X).$$

Under the made assumptions in the Hypotheses and basic definitions we may not proceed as in [16], since this requires at crucial points the point-wise trace-class membership and integrability of $A'(\cdot)\left(A_-^2 + 1\right)^{-1/2}$, which is not available to us. Therefore, we must take a detour to compile the properties of D. To that end, we introduce the operators $H_\pm$ in $L^2(\mathbb{R}, H)$ first, the second central objects of our inquiry in $L^2(\mathbb{R}, H)$.

Definition 2.26. Assume Hypothesis B1 (2.12) or Hypothesis B2 (2.14). Define the operators $M_\pm$ in $L^2(\mathbb{R}, H)$ with domains $\mathrm{Dom}(M_\pm) = \mathrm{Dom}\left(\widehat{A_-^2}\right)$ by

$$M_\pm := A(X)^2 - \widehat{A_-^2} \pm A'(X). \tag{110}$$

Define the operators $H_\pm$ with domains $\mathrm{Dom}(H_\pm) = \mathrm{Dom}(H_0)$ by

$$H_\pm := H_0 + M_\pm. \tag{111}$$

Remark 2.27. The operators $M_\pm$ are well-defined on $\mathrm{Dom}\left(\widehat{A_-^2}\right)$, by either of the Hypotheses B1 (2.12) or B2 (2.14), and therefore also on $\mathrm{Dom}(H_0)$ by Lemma 2.8.

The above Definition 2.26 prompts us at discussing the operators $H_\pm$ as perturbations of H_0. Since the perturbation $M_\pm$ is an operator with domain $\mathrm{Dom}\left(\widehat{A_-^2}\right)$, we see the necessity of including the mapping properties of the operator families $A(x)$, $x \in \mathbb{R}$, and $A'(x)$, $x \in \mathbb{R}$, from $\mathrm{Dom}\left(A_-^2\right)_\Gamma$ to $\mathrm{Dom}(A_-)_\Gamma$ to our Hypotheses in contrast to [16, Hypothesis 2.1] (where only the result $\mathrm{Dom}\left(H_\pm^{1/2}\right) = \mathrm{Dom}\left(H_0^{1/2}\right)$ is needed).

Proposition 2.28. *Assume Hypothesis B1 (*2.12*) or Hypothesis B2 (*2.14*). Then the operators $H_\pm$ are self-adjoint and non-negative. The graph norms of $H_\pm$ and H_0 on* $\mathrm{Dom}(H_0)$ *are equivalent, as well as the graph norms of $H_\pm^{1/2}$, $H_0^{1/2}$ and D_0 on* $\mathrm{Dom}(D_0)$ *are equivalent. Furthermore, the operator D is closed with*

$$\mathrm{Dom}(D) = \mathrm{Dom}(D^*) = \mathrm{Dom}(D_0), \tag{112}$$

where all the respective graph norms are equivalent, and

$$D^*D = H_-, \ DD^* = H_+. \tag{113}$$

Proof. The first part of this proof is in some regard identical to the proof of [16, Lemma 4.4]. However, for the convenience of the reader, we will write it out here with the necessary changes.

We start by assuming Hypothesis B1 (2.12).
Consider the H-valued Fourier transform $\mathcal{F}$ in $L^2(\mathbb{R}, H)$ defined as in [16, (4.33)]. By Lemma 2.8 and via the transform $\mathcal{F}$, the operator H_0 is unitarily equivalent to the operator $X^2 + \widehat{A_-^2}$ in the space $L^2(\mathbb{R}, H)$ with domain

$$\mathrm{Dom}\left(X^2 + \widehat{A_-^2}\right) = \mathrm{Dom}\left(X^2\right) \cap \mathrm{Dom}\left(\widehat{A_-^2}\right). \tag{114}$$

By Lemma 2.44 and the spectral theorem for A_-, we obtain for $z > 0$

$$\begin{aligned} \left\| \left(\widehat{A_-^2} + z\right)(H_0 + z)^{-1} \right\|_{B(L^2(\mathbb{R},H))} &= \sup_{x\in\mathbb{R}} \left\| \left(A_-^2 + z\right)\left(x^2 + A_-^2 + z\right)^{-1} \right\|_{B(H)} \\ &= \sup_{x\in\mathbb{R}} \sup_{\lambda\in\sigma(A_-)} \left| \frac{\lambda^2 + z}{x^2 + \lambda^2 + z} \right| = 1. \end{aligned} \tag{115}$$

We thus estimate for $z > 1$,

$$\begin{aligned}
&\left\| \left(A(X)^2 - \widehat{A_-^2} \pm A'(X) \right) (H_0 + z)^{-1} \right\|_{B(L^2(\mathbb{R},H))} \\
\leq &\left\| \left(A(X)^2 - \widehat{A_-^2} \pm A'(X) \right) \left(\widehat{A_-^2} + z \right)^{-1} \right\|_{B(L^2(\mathbb{R},H))} \left\| \left(\widehat{A_-^2} + z \right) (H_0 + z)^{-1} \right\|_{B(L^2(\mathbb{R},H))} \\
= &\left\| \left(A(X)^2 - \widehat{A_-^2} \pm A'(X) \right) \left(\widehat{A_-^2} + z \right)^{-1} \right\|_{B(L^2(\mathbb{R},H))} \\
\leq &\sup_{x\in\mathbb{R}} \left\| \left(A(x)^2 - A_-^2 \right) \left(A_-^2 + z \right)^{-1} \right\|_{B(H)} + \sup_{x\in\mathbb{R}} \left\| A'(x) \left(A_-^2 + z \right)^{-1} \right\|_{B(H)}. \qquad (116)
\end{aligned}$$

The first summand at the bottom line is less than 1 for $z \gg 1$, while the second summand decays to 0 for $z \to \infty$, thus, by choosing z large enough, we obtain that

$$\left\| \left(A(X)^2 - \widehat{A_-^2} \pm A'(X) \right) (H_0 + z)^{-1} \right\|_{B(L^2(\mathbb{R},H))} < 1, \qquad (117)$$

for $z \gg 1$. In other terms, there exists $1 > \epsilon > 0$ and $\eta > 0$, such that for $f \in \mathrm{Dom}(H_0)$, we have

$$\left\| \left(A(X)^2 - \widehat{A_-^2} \pm A'(X) \right) f \right\|_{L^2(\mathbb{R},H)} \leq \epsilon \|H_0 f\|_{L^2(\mathbb{R},H)} + \eta \|f\|_{L^2(\mathbb{R},H)}. \qquad (118)$$

Thus $A(X)^2 - \widehat{A_-^2} \pm A'(X)$ is relatively bounded with respect to H_0 in $L^2(\mathbb{R}, H)$ with relative bound $\epsilon < 1$. Since H_0 is self-adjoint in $L^2(\mathbb{R}, H)$, also

$$H_\pm = H_0 + A(X)^2 - \widehat{A_-^2} \pm A'(X)$$

must be self-adjoint on $\mathrm{Dom}(H_0)$ by Kato-Rellich's theorem (c.f. [22, Theorem V.4.3]).

Assume now Hypothesis B2 (2.14) instead.
Define the self-adjoint, non-negative operator

$$H_0^B := \left(D_0^B\right)^* D_0^B = D_0^B \left(D_0^B\right)^*, \qquad (119)$$

where $D_0^B := \partial + \widehat{B_0^* A_- B_0}$.[7] Similar to Lemma 2.8 one shows

$$H_0^B = -\partial^2 + (\widehat{B_0^* A_- B_0})^2. \qquad (120)$$

Thus, by the invertibility of B_0, we conclude that $\mathrm{Dom}\left(H_0^B\right)_\Gamma = \mathrm{Dom}(H_0)_\Gamma$.
By Fourier transformation, H_0^B is unitarily equivalent to the operator $X^2 + (\widehat{B_0^* A_- B_0})^2$ in $L^2(\mathbb{R}, H)$. We thus obtain for $z > 0$ by Lemma 2.44,

$$\left\| \left((\widehat{B_0^* A_- B_0})^2 + z \right) \left(H_0^B + z \right)^{-1} \right\|_{B(L^2(\mathbb{R},H))} = \sup_{x\in\mathbb{R}} \sup_{\lambda \in \sigma\left(B_0^* A_- B_0\right)} \left| \frac{\lambda^2 + z}{x^2 + \lambda^2 + z} \right| = 1. \qquad (121)$$

[7]The operator D_0^B has the same properties as D_0 displayed in Lemma 2.6, if A_- is replaced with $B_0^* A_- B_0$. Note also that $\mathrm{Dom}(A_-)_\Gamma = \mathrm{Dom}(B_0^* A_- B_0)_\Gamma$ by the invertibility of B_0.

For $z > 1$ we estimate therefore,

$$\begin{aligned}
&\left\| \left(A(X)^2 - (\widehat{B_0^* A_- B_0})^2 \pm A'(X) \right) \left(H_0^B + z \right)^{-1} \right\|_{B(L^2(\mathbb{R},H))} \\
\leq &\left\| \left(A(X)^2 - (\widehat{B_0^* A_- B_0})^2 \pm A'(X) \right) \left((\widehat{B_0^* A_- B_0})^2 + z \right)^{-1} \right\|_{B(L^2(\mathbb{R},H))} \\
&\left\| \left((\widehat{B_0^* A_- B_0})^2 + z \right) \left(H_0^B + z \right)^{-1} \right\|_{B(L^2(\mathbb{R},H))} \\
= &\left\| \left(A(X)^2 - (\widehat{B_0^* A_- B_0})^2 \pm A'(X) \right) \left((\widehat{B_0^* A_- B_0})^2 + z \right)^{-1} \right\|_{B(L^2(\mathbb{R},H))} \\
\leq &\sup_{x\in\mathbb{R}} \left\| \left(A(x)^2 - (B(x)^* A_- B(x))^2 \right) \left((B_0^* A_- B_0)^2 + z \right)^{-1} \right\|_{B(H)} \\
&+ \sup_{x\in\mathbb{R}} \left\| A'(x) \left((B_0^* A_- B_0)^2 + z \right)^{-1} \right\|_{B(H)} + \sup_{x\in\mathbb{R}} \left\| A'(x) \left((B_0^* A_- B_0)^2 + z \right)^{-1} \right\|_{B(H)} \\
\leq &C z^{-1+\alpha} + \epsilon + \sup_{x\in\mathbb{R}} \left\| A'(x) \left((B_0^* A_- B_0)^2 + z \right)^{-1} \right\|_{B(H)} \\
\xrightarrow{z\to+\infty} &\epsilon < 1.
\end{aligned} \tag{122}$$

We conclude analogous to the case if Hypothesis B1 (2.12) is assumed, that

$$A(X)^2 - (\widehat{B_0^* A_- B_0})^2 \pm A'(X)$$

is relatively bounded with respect to H_0^B with relative bound $\epsilon < 1$. Therefore by Kato-Rellich's theorem (c.f. [22, Theorem V.4.3]), the operator

$$H_\pm = H_0^B + A(X)^2 - (\widehat{B_0^* A_- B_0})^2 \pm A'(X) \tag{123}$$

must be self-adjoint on $\operatorname{Dom}\left(H_0^B\right) = \operatorname{Dom}(H_0)$.

So, if Hypothesis B1 (2.12) or B2 (2.14) is assumed, the graph norms of $H_\pm$ and H_0 are equivalent on $\operatorname{Dom}(H_0)$. Furthermore $H_\pm$ must be essentially self-adjoint on any core of H_0, respectively H_0^B, by Kato-Rellich's theorem ([22, Theorem V.4.3]). We note that

$$C = \bigcup_{n\in\mathbb{N}} \operatorname{rg}\left(\mathbb{1}_{[-n,n]}(\mathbb{i}\partial)\, \mathbb{1}_{[-n,n]}\left(\widehat{A_-} \right) \right) \tag{124}$$

is a core of H_0 and H_0^B, indeed the strong convergence of $\mathbb{1}_{[-n,n]}(\mathbb{i}\partial)\, \mathbb{1}_{[-n,n]}\left(\widehat{A_-} \right)$ to 1 in $L^2(\mathbb{R}, H)$, by functional calculus, shows that for $f \in \operatorname{Dom}(H_0) = \operatorname{Dom}\left(H_0^B\right)$ we have, minding the commutativity of the functional calculi of $H_0, H_0^B, \mathbb{i}\partial$, and $\widehat{A_-}$, that

$$\begin{aligned}
\mathbb{1}_{[-n,n]}(\mathbb{i}\partial)\, \mathbb{1}_{[-n,n]}\left(\widehat{A_-} \right) f &\xrightarrow{n\to\infty} f, \\
H_0 \mathbb{1}_{[-n,n]}(\mathbb{i}\partial)\, \mathbb{1}_{[-n,n]}\left(\widehat{A_-} \right) f = \mathbb{1}_{[-n,n]}(\mathbb{i}\partial)\, \mathbb{1}_{[-n,n]}\left(\widehat{A_-} \right) H_0 f &\xrightarrow{n\to\infty} H_0 f,
\end{aligned} \tag{125}$$

which means that C is dense in $\mathrm{Dom}\,(H_0)_\Gamma = \mathrm{Dom}\,\left(H_0^B\right)_\Gamma$, and is therefore a core of H_0 and H_0^B.

For the second part of the proof define

$$D_- := -\partial + A\,(X)\,, \quad D_+ := D, \quad \mathrm{Dom}\,(D_\pm) := \mathrm{Dom}\,(D_0)\,. \tag{126}$$

For $f, g \in \mathrm{Dom}\,(D_0)$ we have

$$\langle D_- f, g\rangle_{L^2(\mathbb{R},H)} = \langle f, D_+ g\rangle_{L^2(\mathbb{R},H)}. \tag{127}$$

Thus for $g \in \mathrm{Dom}\,(D_0)$ we have that

$$f \mapsto \langle D_- f, g\rangle_{L^2(\mathbb{R},H)} = \langle f, D_+ g\rangle_{L^2(\mathbb{R},H)}, \tag{128}$$

is an $L^2\,(\mathbb{R}, H)$-continuous functional on $\mathrm{Dom}\,(D_-) = \mathrm{Dom}\,(D_0)$, and therefore $g \in \mathrm{Dom}\,\left(D_-^*\right)$. So $\mathrm{Dom}\,(D_0) \subseteq \mathrm{Dom}\,\left(D_-^*\right)$ and analogously we conclude $\mathrm{Dom}\,(D_0) \subseteq \mathrm{Dom}\,\left(D_+^*\right)$. Since $\mathrm{Dom}\,(D_0)$ is dense, the adjoints $D_\mp^*$ must be densely defined. Thus $D_\pm$ are closable operators in $L^2\,(\mathbb{R}, H)$. We may construct

$$\widetilde{H_-} := D_+^* \overline{D_+}, \quad \widetilde{H_+} := D_-^* \overline{D_-}, \tag{129}$$

which are automatically self-adjoint, non-negative operators in $L^2\,(\mathbb{R}, H)$ with dense domains and we have

$$\left|\overline{D_\pm}\right| = \widetilde{H_\mp}^{1/2}. \tag{130}$$

However, for $f \in C$, we have $H_\pm f = \widetilde{H_\pm} f$. Since $H_\pm$ is essentially self-adjoint on C, we conclude that $H_\pm = \widetilde{H_\pm}$ and thus the operators $H_\pm$ are non-negative as well. But then Lemma 2.21 also implies that $\mathrm{Dom}\left(H_\pm^{1/2}\right)_\Gamma = \mathrm{Dom}\left(H_0^{1/2}\right)_\Gamma = \mathrm{Dom}\,(D_0)_\Gamma$ holds. Therefore we get the following continuous (with respect to the graph norms) inclusions

$$\mathrm{Dom}\,(D_0) \subseteq \mathrm{Dom}\,\left(\overline{D_\pm}\right) = \mathrm{Dom}\,\left(\left|\overline{D_\pm}\right|\right) = \mathrm{Dom}\left(H_\mp^{1/2}\right) = \mathrm{Dom}\,(D_0)\,. \tag{131}$$

Summarily $\overline{D} = \overline{D_+} = D_+ = D$ and $D^* = D_+^* = \overline{D_-} = D_-$ holds and $\mathrm{Dom}\,(D^*)_\Gamma = \mathrm{Dom}\,(D_0)_\Gamma = \mathrm{Dom}\,(D)_\Gamma$. ■

A first consequence of the above Proposition 2.28 is the following version of Duhamel's formula (sometimes also referred to as the (induction step of the) Volterra series) for the operators $H_\pm$, which is our basic tool in discussing perturbations of semi-groups, and can therefore be considered as the "analogue" of the resolvent identities.

Lemma 2.29. *Let $t_0 \geq t > 0$. Then*

$$e^{-tH_\pm} - e^{-tH_0} = -\int_0^t e^{-sH_\pm} M_\pm e^{-(t-s)H_0} \mathrm{d}s = -\int_0^t e^{-sH_0} M_\pm e^{-(t-s)H_\pm} \mathrm{d}s. \tag{132}$$

The integrals converge in $B\left(L^2\,(\mathbb{R}, H)\right)$-norm and for $\alpha \in [0,1]$ and $t_0 \geq t > s > 0$

$$\begin{aligned} \left\| e^{-sH_\pm} M_\pm e^{-(t-s)H_0} \right\|_{B(L^2(\mathbb{R},H))} &\lesssim_{t_0} s^{-\alpha}\,(t-s)^{-1+\alpha}\,, \\ \left\| e^{-sH_0} M_\pm e^{-(t-s)H_\pm} \right\|_{B(L^2(\mathbb{R},H))} &\lesssim_{t_0} s^{-\alpha}\,(t-s)^{-1+\alpha}\,. \end{aligned} \tag{133}$$

Proof. We only prove the first equality of (132) and the first inequality of (133), since the second ones are proven analogously.

Before we show equality in (132), we have to make sure that the integrand exists as a bounded operator valued, integrable function in s. We first note that for $0 < s < t$ the operator $e^{-(t-s)H_0}$ maps $L^2(\mathbb{R}, H)$ continuously into $\mathrm{Dom}(H_0)$, which is continuously embedded in $\mathrm{Dom}\left(\widehat{A_-^2}\right)$, by Lemma 2.8. Hence, the integrand of (132) is a bounded operator. Furthermore, we note that the integrand is $B\left(L^2(\mathbb{R}, H)\right)$-norm continuous for $s \in (0,t)$, by Lemma 2.37, and thus $B\left(L^2(\mathbb{R}, H)\right)$-measurable in s. For $\alpha \in [0,1]$ the norm of the integrand can be estimated by

$$\begin{aligned}
&\left\| e^{-sH_\pm} M_\pm e^{-(t-s)H_0} \right\|_{B(L^2(\mathbb{R},H))} \\
&= \Big\| \left(e^{-sH_\pm} (H_\pm + 1)^\alpha\right) \left((H_\pm + 1)^{-\alpha} (H_0 + 1)^\alpha\right) \left((H_0 + 1)^{-\alpha} M_\pm (H_0 + 1)^{-1+\alpha}\right) \\
&\qquad \left((H_0 + 1)^{1-\alpha} e^{-(t-s)H_0}\right) \Big\|_{B(L^2(\mathbb{R},H))} \\
&\lesssim_{t_0} s^{-\alpha} \cdot \left\| \left\{ (H_0 + 1)^{-\alpha} M_\pm (H_0 + 1)^{-1+\alpha} \right\} \right\|_{B(L^2(\mathbb{R},H))} \cdot (t-s)^{-1+\alpha} \\
&\lesssim_{t_0} s^{-\alpha} (t-s)^{-1+\alpha}, \qquad (134)
\end{aligned}$$

which is inequality (133). Here we used Lemma 2.21, Remark 2.20, and Corollary 2.39. For $\alpha \in (0,1)$, the norm is integrable in s on $[0,t]$ and the (Bochner-) integral therefore converges in $B\left(L^2(\mathbb{R}, H)\right)$ by Lemma 2.41.
We are left with showing the claimed equality (132). Let $f \in L^2(\mathbb{R}, H)$. Then $e^{-(t-s)H_0} f \in \mathrm{Dom}(H_0)$, for $s < t$. On $\mathrm{Dom}(H_0)$ the equality $H_\pm = H_0 + M_\pm$ holds by Definition 2.26. We may conclude

$$\begin{aligned}
-\int_0^t e^{-sH_\pm} M_\pm e^{-(t-s)H_0} \mathrm{d}s\, f &= -\int_0^t e^{-sH_\pm} (H_\pm - H_0) e^{-(t-s)H_0} f \mathrm{d}s \\
&= \int_0^t \partial_s \left(e^{-sH_\pm} e^{-(t-s)H_0} f\right) \mathrm{d}s \\
&= \left[e^{-sH_\pm} e^{-(t-s)H_0} f\right]_{s=0}^{s=t} = \left(e^{-tH_\pm} - e^{-tH_0}\right) f. \qquad (135)
\end{aligned}$$

Here we used the well-known strong continuity of one-parameter semi-groups on closed intervals and differentiability on open intervals. ■

Let us proceed by introducing some auxiliary operators, which will play a central role in calculating the trace formulae.

Definition 2.30. Assume Hypothesis B1 (2.12) or Hypothesis B2 (2.14) and let $t > 0$. We define the bounded operator in $L^2(\mathbb{R}, H)$

$$P_t^+ := D^* e^{-tH_+}. \qquad (136)$$

Remark 2.31. Since for $t > 0$ the operator e^{-tH_+} maps $L^2(\mathbb{R}, H)$ continuously into $\mathrm{Dom}(H_0)_\Gamma$, and $\mathrm{Dom}(D^*) = \mathrm{Dom}\left(H_0^{1/2}\right)$, by Proposition 2.28, the operator P_t^+ is indeed bounded in $L^2(\mathbb{R}, H)$.

The relevance of the operator P_t^+ stems from the following identity involving a commutator with ∂.

Lemma 2.32. *Assume Hypothesis B1 (*2.12*) or Hypothesis B2 (*2.14*) and let* $t > 0$. *Then*

$$H_+ e^{-tH_+} - H_- e^{-tH_-} = \left\{ \left[\partial, P_t^+ \right] \right\} + \left\{ \left[A(X), P_t^+ \right] \right\}. \tag{137}$$

Proof. By Lemma 2.40 we have for $f \in \mathrm{Dom}(D_0)$,

$$\begin{aligned} H_+ e^{-tH_+} f - H_- e^{-tH_-} f &= DD^* e^{-tH_+} f - D^* e^{-tH_+} Df = DP_t^+ f - P_t^+ Df \\ &= \left[\partial, P_t^+ \right] f + \left[A(X), P_t^+ \right] f. \end{aligned} \tag{138}$$

Furthermore $P_t^+ \partial$ is a closable operator in $L^2(\mathbb{R}, H)$, and

$$P_t^+ \partial f = P_{t/2}^+ e^{-t/2 H_+} \partial f = P_{t/2}^+ \left\{ e^{-t/2 H_+} \partial \right\} f, \tag{139}$$

where the right hand side exists by Proposition 2.28 and Lemma 2.19 as a bounded operator in $L^2(\mathbb{R}, H)$ applied to f. Therefore also $\left\{ P_t^+ \partial \right\}$ and hence $\left\{ \left[\partial, P_t^+ \right] \right\}$ exist. For the existence of $\left\{ \left[A(X), P_t^+ \right] \right\}$ we argue similarly.
Thus equation (138) extends by continuity and density of $\mathrm{Dom}(D_0)$ in $L^2(\mathbb{R}, H)$ to

$$H_+ e^{-tH_+} - H_- e^{-tH_-} = \left\{ \left[\partial, P_t^+ \right] \right\} + \left\{ \left[A(X), P_t^+ \right] \right\}. \tag{140}$$

■

Because the operator P_t^+ is connected to the difference $H_+ e^{-tH_+} - H_- e^{-tH_-}$, we close this subsection by introducing another operator in $L^2(\mathbb{R}, H)$, which is connected to the difference $e^{-tH_+} - e^{-tH_-}$, which will be discussed in more detail in Theorem 3.22.

Definition 2.33. For $z \in \mathbb{C}$, let

$$\gamma(z) := \sum_{k=0}^{\infty} \frac{1}{(k+1)!} (-z)^k = \begin{cases} \frac{1-e^{-z}}{z}, & z \neq 0, \\ 1, & z = 0. \end{cases} \tag{141}$$

γ is an entire function and bounded on $\{z \in \mathbb{R},\ z \geq 0\}$. Define the bounded operator Q_t^+ in $L^2(\mathbb{R}, H)$ by

$$Q_t^+ := D^* \gamma(tH_+). \tag{142}$$

Remark 2.34. For $z \in \mathbb{C}$ and $t > 0$, we have $\gamma(tz)(1+z) = \gamma(tz) + t^{-1}\left(1 - e^{-tz}\right)$, and thus

$$\gamma(tH_\pm) = (1 + H_\pm)^{-1} \left(\gamma(tH_\pm) + t^{-1} \left(1 - e^{-tH_\pm} \right) \right). \tag{143}$$

Hence, the operators $\gamma(tH_\pm)$ map $L^2(\mathbb{R}, H)$ continuously into $\mathrm{Dom}(H_0)_\Gamma$, by Proposition 2.28, and the operator Q_t^+ is indeed bounded in $L^2(\mathbb{R}, H)$.

In the next subsection, the last of this chapter, we compile all remaining basic tools and definitions needed for the chapters to come.

2.5 Auxiliary definitions and facts

The purpose of this subsection is to provide the remaining miscellaneous definitions and well-known facts, which will be needed in this work, but do not quite fit in some of the other introductory subsections or rise to the complexity of requiring their own subsection.

We begin by introducing the Gauss kernel, which we will repeatedly use.

Definition 2.35. Let $t > 0$. We define q_t to be the Gauss kernel, i.e. for $x \in \mathbb{R}$,

$$q_t(x) := (4\pi t)^{-1/2} e^{-\frac{x^2}{4t}}. \tag{144}$$

Without proof, we cite some well-known facts of the Gauss kernel. They can be shown by standard integration techniques.

Lemma 2.36. *For $t > 0$ the function $(x, y) \mapsto q_t(x - y)$ is a smooth integral kernel of the operator $e^{t\partial_{\mathbb{C}}^2}$ in $L^2(\mathbb{R})$, i.e. for $f \in L^2(\mathbb{R})$*

$$\left(e^{t\partial_{\mathbb{C}}^2} f\right)(x) = \int_{\mathbb{R}} q_t(x - y) f(y)\, \mathrm{d}y, \text{ for (a.e.) } x \in \mathbb{R}. \tag{145}$$

Let $t > 0$ and $1 \le p < \infty$, then

$$\begin{aligned} \|q_t\|_{L^p(\mathbb{R})} &= (4\pi)^{\frac{1}{2p}-\frac{1}{2}} p^{-\frac{1}{2p}} t^{\frac{1}{2p}-\frac{1}{2}}, \\ \|q_t'\|_{L^p(\mathbb{R})} &= (4\pi)^{-1/2} \left(2\,\Gamma\left(\frac{p+1}{2}\right)\right)^{1/p} p^{-\frac{1}{2}-\frac{1}{2p}} t^{\frac{1}{2p}-1}. \end{aligned} \tag{146}$$

The next simple result extends the well-known strong continuity of semi-groups to norm continuity on open intervals.

Lemma 2.37. *Let T be a linear, (unbounded), non-negative operator in a Hilbert space X. Then $s \mapsto e^{-sT}$ is $B(X)$-norm continuous for $s > 0$.*

Proof. Let $\epsilon > 0$. Let $0 < r < s, t$. Let $R \gg 0$, such that $e^{-R} \le \epsilon/2$, and let $\delta > 0$ be small enough such that

$$1 - e^{-r^{-1}R\delta} \le \epsilon/2. \tag{147}$$

Then, for $|s - t| \le \delta$, we find

$$\begin{aligned} \left\|e^{-sT} - e^{-tT}\right\|_{B(X)} &= \left\|e^{-\min(s,t)T}\left(1 - e^{-|s-t|T}\right)\right\|_{B(X)} \\ &\le \sup_{\lambda \ge 0} \left|e^{-r\lambda}\left(1 - e^{\delta\lambda}\right)\right| \\ &\le \sup_{\lambda \ge r^{-1}R} \left|e^{-r\lambda}\right| + \sup_{r^{-1}R > \lambda \ge 0} \left|1 - e^{\delta\lambda}\right| \\ &\le \epsilon/2 + \epsilon/2. \end{aligned} \tag{148}$$

■

The next estimate allows us to calculate the norm of semi-groups in domains of the powers of the generating operator.

Lemma 2.38. *Let $t > 0$, $\beta \geq 0$. Then*

$$\sup_{u\geq 0} (u+1)^{\beta} e^{-tu} = \begin{cases} \left(\frac{\beta}{et}\right)^{\beta} e^{t} & \text{if } t \leq \beta, \\ 1 & \text{if } t > \beta, \end{cases}$$
$$\leq \left(\frac{\beta}{et}\right)^{\beta} e^{t}. \tag{149}$$

Proof. Put $\phi(u) := (u+1)^{\beta} e^{-tu}$. Since

$$\lim_{u\to\infty} \phi(u) = 0,$$
$$\phi(0) = 1, \tag{150}$$

we only need to check for local extrema of ϕ on $\{x \in \mathbb{R},\ x > 0\}$. The extremum lies at $u_0 = \beta t^{-1} - 1$, hence is only present in case $\beta \geq t$. In this case we find

$$\phi(u_0) = \left(\frac{\beta}{et}\right)^{\beta} e^{t}. \tag{151}$$

The expression $\left(\frac{\beta}{et}\right)^{\beta} e^{t}$, as a function of t, diverges to $+\infty$ for $t \to 0+$ and $t \to +\infty$. Its extremum lies at $t_0 = \beta$, for which $\left(\frac{\beta}{et_0}\right)^{\beta} e^{t_0} = 1$. Thus, for all $t > 0$ we have $\left(\frac{\beta}{et}\right)^{\beta} e^{t} \geq 1$, which finishes the proof. ■

Corollary 2.39. *Let $0 < t \leq t_0$ and $\beta \geq 0$. Let T be a linear, self-adjoint, non-negative operator in a Hilbert space X. Then*

$$\left\| (T+1)^{\beta} e^{-tT} \right\|_{B(H)} \lesssim_{t_0,\beta} t^{-\beta}. \tag{152}$$

Proof. The result follows directly from Lemma 2.38 and the functional calculus of T. ■

The following Lemma 2.40 provides some commutation relations for the operators D, D^*, and $H_{\pm}$.

Lemma 2.40. *Let ϕ be a continuous, bounded function on $\{x \in \mathbb{R},\ x \geq 0\}$ and let $f \in$ $\mathrm{Dom}(D_0)$. Then*

$$D^{*}\phi(H_{+}) f = \phi(H_{-}) D^{*} f,$$
$$D\phi(H_{-}) f = \phi(H_{+}) Df. \tag{153}$$

Proof. Let $(0,1] \ni x \mapsto \psi(x) := x^{-1} - 1 \in \{y \in \mathbb{R},\ y \geq 0\}$ and $\psi(0) := +\infty$, then $\phi \circ \psi \in C([0,1])$. By the Stone-Weierstrass theorem there exists a sequence of polynomials

$p_n \in \mathbb{C}[X]$, which uniformly converges to $\phi \circ \psi$ on $[0,1]$.
Let $f \in \operatorname{Dom}(D_0)$ and let $g := (1+H_+)^{-1} f$, then

$$\begin{aligned}(1+H_-)^{-1} D^* f &= (1+H_+)^{-1} D^* (DD^* + 1) g \\ &= (1+H_+)^{-1} (D^* D + 1) D^* g = D^* g \\ &= D^* (1+H_+)^{-1} f. \end{aligned} \tag{154}$$

Similarly one shows

$$(1+H_+)^{-1} Df = D (1+H_-)^{-1} f. \tag{155}$$

Thus we have for any polynomial $p \in \mathbb{C}[X]$

$$\begin{aligned} p\left((1+H_-)^{-1}\right) D^* f = D^* p\left((1+H_+)^{-1}\right) f, \\ p\left((1+H_+)^{-1}\right) Df = Dp\left((1+H_-)^{-1}\right) f. \end{aligned} \tag{156}$$

The continuous functional calculus therefore implies, for $f, g \in \operatorname{Dom}(D_0)$,

$$\begin{aligned} \langle g, \phi(H_-) D^* f \rangle_{L^2(\mathbb{R},H)} &= \langle g, (\phi \circ \psi)\left((1+H_-)^{-1}\right) D^* f \rangle_{L^2(\mathbb{R},H)} \\ &= \lim_{n\to\infty} \langle g, p_n \left((1+H_-)^{-1}\right) D^* f \rangle_{L^2(\mathbb{R},H)} \\ &= \lim_{n\to\infty} \langle g, D^* p_n \left((1+H_+)^{-1}\right) f \rangle_{L^2(\mathbb{R},H)} \\ &= \langle Dg, \phi(H_+) f \rangle_{L^2(\mathbb{R},H)} \\ &= \langle g, D^* \phi(H_+) f \rangle_{L^2(\mathbb{R},H)}. \end{aligned} \tag{157}$$

In the last step, we used that the operator $\phi(H_+)$ maps $\operatorname{Dom}(D_0)_\Gamma$ continuously into itself, since $\operatorname{Dom}(D_0)_\Gamma = \operatorname{Dom}\left(H_\pm^{1/2}\right)$, by Proposition 2.28. By density of $\operatorname{Dom}(D_0)$ in $L^2(\mathbb{R}, H)$, and the afore mentioned continuity, we obtain

$$D^* \phi(H_+) f = \phi(H_-) D^* f. \tag{158}$$

Similarly one obtains

$$D\phi(H_-) f = \phi(H_+) Df. \tag{159}$$

■

Without proof, we also cite [16, Lemma 3.1] which summarizes the Bochner theorem in the case of trace-class operators and their Radon-Nikodym property.

Lemma 2.41. *Let X be a complex, separable Hilbert-space and $F(x)$, $x \in \mathbb{R}$, a family of trace-class operators in X. Then the following assertions (1) and (2) are equivalent:*

1. *$F(x)$, $x \in \mathbb{R}$, is a weakly measurable family of operators in $B(X)$ and $\|F(\cdot)\|_{S^1(X)} \in L^1(\mathbb{R})$.*

2. *$F(\cdot) \in L^1(\mathbb{R}, S^1(X))$.*
Moreover if either condition (1) or (2) holds, then

$$\left\| \int_{\mathbb{R}} F(x)\,\mathrm{d}x \right\|_{S^1(X)} \le \int_{\mathbb{R}} \|F(x)\|_{S^1(X)}, \tag{160}$$

and the $S^1(X)$-valued function

$$\mathbb{R} \ni x \mapsto \int_{x_0}^{x} F(y)\,\mathrm{d}y, \quad x_0 \in \mathbb{R} \cup \{-\infty\}, \tag{161}$$

is strongly absolutely continuous with respect to the norm in $S^1(X)$.
In addition we recall the following fact:

3. *Suppose that $\mathbb{R} \ni x \mapsto G(x) \in S^1(X)$ is strongly locally absolutely continuous in $S^1(X)$. Then $H(x) = G'(x)$ exists for a.e. $x \in \mathbb{R}$, $H(\cdot)$ is Bochner integrable over any compact interval, and hence*

$$G(x) = G(x_0) + \int_{x_0}^{x} H(y)\,\mathrm{d}y, \quad x, x_0 \in \mathbb{R}, \tag{162}$$

where the integral converges in $S^1(X)$.

Finally, let us deal with the notion of N-measurability, which is assumed in the definition 2.3 of the family $A(x)$, $x \in \mathbb{R}$, and $A'(x)$, $x \in \mathbb{R}$. We summarize the most important properties presented in [16, Appendix A].

Definition 2.42. A family $T(x)$, $x \in \mathbb{R}$, of linear, closed operators in H is N-measurable, if the families

$$(|T(x)| + 1)^{-1},\ T(x)(|T(x)| + 1)^{-1},\ \text{and}\ (|T(x)^*| + 1)^{-1},\ x \in \mathbb{R},$$

are weakly measurable. A family $S(x)$, $x \in \mathbb{R}$, is weakly measurable, if for any weakly measurable family $f(x)$, $x \in \mathbb{R}$, in H, such that $f(x) \in \mathrm{Dom}(S(x))$ for $x \in \mathbb{R}$, the family of elements $S(x)f(x)$, $x \in \mathbb{R}$, is weakly measurable in H. Finally, a family $g(x)$, $x \in \mathbb{R}$, is weakly measurable in H, if for any $\phi \in H$ the family $\langle \phi, g(x) \rangle_H$, $x \in \mathbb{R}$ is Lebesgue measurable over $\mathbb{R}$.

Remark 2.43. The above Definition 2.42 is a compilation of [16, Definition A.3] and [16, Remark A.4], especially statement [16, (A.10)] in [16, Appendix A].

Lemma 2.44. *(Nussbaum, [29]) Assume that $T(x)$, $x \in \mathbb{R}$, is a N-measurable family of densely defined, closed , linear operators in H. Then the following assertions hold:*

1. *$T(X)$ is densely defined and closed in $L^2(\mathbb{R}, H)$ and $(T(X))^* = T^*(X)$, $|T(X)| = |T|(X)$.*

2. *$T(X)$ is symmetric (respectively self-adjoint, or normal) in $L^2(\mathbb{R}, H)$ if and only if $T(x)$ is symmetric (respectively self-adjoint, or normal) in H for a.e. $x \in \mathbb{R}$.*

3. *If $T(X)$ is self-adjoint in $L^2(\mathbb{R}, H)$, then $T(X) \geq 0$ if and only if $T(x) \geq 0$ for a.e. $x \in \mathbb{R}$.*

4. *If $T(X)$ is normal in $L^2(\mathbb{R}, H)$, then $p(T(X)) = p(T)(X)$ for any polynomial p.*

5. *If $S(x)$, $x \in \mathbb{R}$, are densely defined, closed, linear operators in H and $S(x)$, $x \in \mathbb{R}$, is N-measurable, then $T(X) \subseteq S(X)$ if and only if $T(x) \subseteq S(x)$ for a.e. $x \in \mathbb{R}$.*

6. *If $T(x) \in B(H)$ for $x \in \mathbb{R}$, then $T(X) \in B\left(L^2(\mathbb{R}, H)\right)$ if and only if $\operatorname{ess\,sup}_{x \in \mathbb{R}} \|T(x)\|_{B(H)} < \infty$. In particular under this assumption we have $\|T(X)\|_{B(L^2(\mathbb{R},H))} = \operatorname{ess\,sup}_{x \in \mathbb{R}} \|T(x)\|_{B(H)}$.*

Remark 2.45. The above Lemma 2.44 comprises of [16, Theorem A.7], which in turn stems from [29], and the statements [16, (A.18)] and [16, (A.19)].

The Remark 2.45 above closes this subsection and hence the first chapter, which sets the scene for this work, by introducing all the involved operators, and reviewing their basic properties, which are not related to the trace-class. In the next chapter, we will deal with exactly this so far omitted point of view for the introduced operators in H and $L^2(\mathbb{R}, H)$.

3 Trace-class memberships

In this chapter we will discuss the trace-class properties of several operators related to the family $A(x)$, $x \in \mathbb{R}$ in H and the operators D, $H_\pm$, and H_0 in $L^2(\mathbb{R}, H)$. While we will also present some results involving resolvents of operators, our methods deviate largely from the techniques used in [16], for example we will not use the double operator integral calculus, which is deployed in [16].

The first subsection 3.1 deals with trace-class memberships of operators in H, which are derived from the family $A(x)$, $x \in \mathbb{R}$. We also give estimates on their trace-norms, which have the purpose of enabling us to extend integral formulas, stemming from Duhamel's formula, to retain convergence in the trace-class.

These results allow us to construct spectral shift functions of the pair (A_+, A_-) in subsection 3.2, where one construction uses a result of Koplienko [24].

Analogous to the first subsection, we discuss in subsection 3.3 the trace-class memberships of certain operators in $L^2(\mathbb{R}, H)$, which are related to the operators D, D_0, and $H_\pm, H_0$. Especially we show the trace-class memberships of the differences

$$\begin{aligned} e^{-tH_+} - e^{-tH_-} &\in S^1\left(L^2(\mathbb{R}, H)\right),\ t > 0, \\ H_+ e^{-tH_+} - H_- e^{-tH_-} &\in S^1\left(L^2(\mathbb{R}, H)\right),\ t > 0, \end{aligned} \tag{163}$$

which form the left hand side of the trace formulae (1) presented in the introduction.

We close the chapter in subsection 3.4 by using the trace-class memberships in the previous subsection 3.3 to construct the spectral shift function of the pair (H_+, H_-).

3.1 Operators in $S^1(H)$

We start by giving the first simple result, which is a direct consequence of Hypothesis A1 (2.10), and Hypothesis A2 (2.11) respectively.

Lemma 3.1. *Assume Hypothesis A1 (*2.10*). Then for $s, t > 0$ and $x \in \mathbb{R} \cup \{\pm\infty\}$ the operator*

$$e^{-tA_-^2}(A(x) - A_-)\, e^{-sA_-^2}$$

is a trace-class operator in H and

$$\sup_{y \in \mathbb{R}} \left\| e^{-tA_-^2}(A(y) - A_-)\, e^{-sA_-^2} \right\|_{S^1(H)} \in I^{log}_{-1/4,-1/4}. \tag{164}$$

If we additionally assume Hypothesis A2 2.11*, then*

$$\sup_{y \in \mathbb{R}} \left\| e^{-tA_-^2}(A(y) - A_-)\, e^{-sA_-^2} \right\|_{S^1(H)} \in I^{log}_{-3/4,-1/4} \cap I^{log}_{-1/4,-3/4}. \tag{165}$$

Proof. For $s, t > 0$ the family $\mathbb{R} \ni y \mapsto e^{-tA_-^2} A'(y)\, e^{-sA_-^2}$ is weakly integrable over $(-\infty, x)$, and thus the integral,

$$\int_{-\infty}^{x} \langle \phi, e^{-tA_-^2} A'(y)\, e^{-sA_-^2} \psi \rangle_H \mathrm{d}y,\ \phi, \psi \in H, \tag{166}$$

exists. The integral (166) converges in the weak operator topology to the operator in question, $e^{-tA_-^2}(A(x)-A_-)e^{-sA_-^2}$. On the other hand, Hypothesis A1 (2.10), respectively Hypothesis (2.11), together with Lemma 2.41, show us that the above integral (166) must also converge in $S^1(H)$ to the same limit. The norm estimates then also directly follow from Lemma 2.41 and the Hypotheses A1 (2.10) or A2 (2.11). ∎

Remark 3.2. Lemma 3.1 immediately implies that for $s,t>0$ and $x\in\mathbb{R}\cup\{\pm\infty\}$ the operator

$$e^{-tA_-^2}(A_+-A(x))e^{-sA_-^2}$$

is a trace-class operator in H, and

$$\sup_{y\in\mathbb{R}}\left\|e^{-tA_-^2}(A_+-A(y))e^{-sA_-^2}\right\|_{S^1(H)}\in I^{log}_{-1/4,-1/4}. \tag{167}$$

If we additionally assume Hypothesis A2 2.11, then

$$\sup_{y\in\mathbb{R}}\left\|e^{-tA_-^2}(A_+-A(y))e^{-sA_-^2}\right\|_{S^1(H)}\in I^{log}_{-3/4,-1/4}\cap I^{log}_{-1/4,-3/4}. \tag{168}$$

By virtue of Lemma 3.1, we can derive the trace-class membership of an expression involving the resolvent of A_-^2, via the Laplace-transform.

Lemma 3.3. *Assume Hypothesis A1 (2.10). Then for $x\in\mathbb{R}\cup\{\pm\infty\}$ the operator*

$$\left(1+A_-^2\right)^{-3/4}(A(x)-A_-)\left(1+A_-^2\right)^{-3/4}$$

is trace-class in H. If we additionally assume Hypothesis A2 (2.11), the operators

$$\begin{gathered}\left(1+A_-^2\right)^{-1/4}(A(x)-A_-)\left(1+A_-^2\right)^{-3/4},\\ \left(1+A_-^2\right)^{-3/4}(A(x)-A_-)\left(1+A_-^2\right)^{-1/4}\end{gathered}$$

are trace-class in H. We also have the estimates

$$\begin{gathered}\left\|\left(1+A_-^2\right)^{-3/4}(A(y)-A_-)\left(1+A_-^2\right)^{-3/4}\right\|_{S^1(H)}\leq F(y),\\ \textit{if Hypothesis A1 (2.10) is assumed,}\\ \left\|\left(1+A_-^2\right)^{-1/4}(A(y)-A_-)\left(1+A_-^2\right)^{-3/4}\right\|_{S^1(H)}\\ +\left\|\left(1+A_-^2\right)^{-3/4}(A(y)-A_-)\left(1+A_-^2\right)^{-1/4}\right\|_{S^1(H)}\leq G(y),\\ \textit{if Hypothesis A2 (2.11) is assumed,}\\ \textit{where } F(y)=\int_{-\infty}^{y}f(z)\,\mathrm{d}z,\ G(y)=\int_{-\infty}^{y}g(z)\,\mathrm{d}z, \textit{ for some } f,g\in L^1(\mathbb{R}).\end{gathered} \tag{169}$$

Furthermore we have the estimates

$$\left\|\left(1+A_-^2\right)^{-3/4}(A_+-A(y))\left(1+A_-^2\right)^{-3/4}\right\|_{S^1(H)}\leq\widetilde{F}(y),$$

if Hypothesis A1 (2.10) is assumed,

$$\left\| \left(1 + A_-^2\right)^{-1/4} \left(A_+ - A(y)\right) \left(1 + A_-^2\right)^{-3/4} \right\|_{S^1(H)} + \left\| \left(1 + A_-^2\right)^{-3/4} \left(A_+ - A(y)\right) \left(1 + A_-^2\right)^{-1/4} \right\|_{S^1(H)} \leq \widetilde{G}(y),$$

if Hypothesis A2 (2.11) is assumed,

$$\textit{where } \widetilde{F}(y) = \int_y^{+\infty} f(z)\,\mathrm{d}z, \ \widetilde{G}(y) = \int_y^{+\infty} g(z)\,\mathrm{d}z, \textit{ for some } f, g \in L^1(\mathbb{R}). \tag{170}$$

Proof. By functional calculus we conclude that for $a > 0$

$$\left(1 + A_-^2\right)^{-a} = \frac{1}{\Gamma(a)} \int_0^\infty e^{-rA_-^2} e^{-r} r^{a-1} \mathrm{d}r, \tag{171}$$

where the integral converges in the strong operator topology. Thus we have for $a, b > 0$,

$$\begin{aligned} &\left(1 + A_-^2\right)^{-a} \left(A(x) - A_-\right) \left(1 + A_-^2\right)^{-b} \\ =&\frac{1}{\Gamma(a)\Gamma(b)} \int_0^\infty \int_0^\infty e^{-r} e^{-s} r^{a-1} s^{b-1} e^{-rA_-^2} \left(A(x) - A_-\right) e^{-sA_-^2} \mathrm{d}s \ \mathrm{d}r. \end{aligned} \tag{172}$$

If we assume Hypothesis A1 (2.10), Lemma 3.1 allows us to conclude that the integrand in (172) is trace-class in H and continuous in r and s from $(0, \infty)^2$ to $S^1(H)$ and is therefore $S^1(H)$-measurable in r and s. Let

$$g(r, s) := \left\| e^{-rA_-^2} \left(A(x) - A_-\right) e^{-sA_-^2} \right\|_{S^1(H)}, \tag{173}$$

then we find for $t_0 > 0$,

$$\begin{aligned} &\int_0^\infty \int_0^\infty e^{-r} e^{-s} r^{a-1} s^{b-1} g(r, s) \,\mathrm{d}s \ \mathrm{d}r \\ \leq &\int_0^{t_0} \int_0^{t_0} e^{-r} e^{-s} r^{a-1} s^{b-1} g(r, s) \,\mathrm{d}s \ \mathrm{d}r + \int_0^{t_0} \int_{t_0}^\infty e^{-r} e^{-s} r^{a-1} s^{b-1} g(r, t_0) \,\mathrm{d}s \ \mathrm{d}r \\ &+ \int_{t_0}^\infty \int_0^{t_0} e^{-r} e^{-s} r^{a-1} s^{b-1} g(t_0, s) \,\mathrm{d}s \ \mathrm{d}r + \int_{t_0}^\infty \int_{t_0}^\infty e^{-r} e^{-s} r^{a-1} s^{b-1} g(t_0, t_0) \,\mathrm{d}s \ \mathrm{d}r \\ <&\infty, \end{aligned} \tag{174}$$

for $a, b = 3/4$, if we assume Hypothesis A1 (2.10), and for $a = 1/4$, $b = 3/4$ or $a = 3/4$, $b = 1/4$, if we assume Hypothesis A2 (2.11), which we conclude by Lemma 3.1. Therefore the integrand in (172) is $S^1(H)$-(Bochner) integrable by Lemma 2.41 and hence the left hand side of (172) is trace-class in H as well, for the appropriate choices of a and b.
Finally, we obtain the estimates (169) by taking the supremum in (174) and minding the estimates from Lemma 3.1.
The estimates (170) are obtained analogously by the use of Remark 3.2. ■

The above Lemma 3.3 is essential in constructing spectral shift functions of the pair (A_+, A_-) due to an approach of Koplienko [24], which uses powers of resolvents. In the next Lemma, we discuss the trace-class properties of $A'(x)\,A(x)$, $x \in \mathbb{R}$, and $A(x)\,A'(x)$, $x \in \mathbb{R}$. This consideration is owed to the fact that we will discuss $H_\pm$ as perturbations of H_0 in $L^2(\mathbb{R}, H)$, and the perturbation $M_\pm$ contains multiplication with the family $A^2(x)$, $x \in \mathbb{R}$. In subsection 3.3 we will deal with commutators of the operator ∂, which, if applied to $A^2(X)$, give multiplication with the two mentioned operator families.

Lemma 3.4. *Assume Hypothesis A2 (*2.11*) and let* $r, s > 0$*. Then* $e^{-rA_-^2} A(x)\,A'(x)\,e^{-sA_-^2}$, $x \in \mathbb{R}$*, and* $e^{-rA_-^2} A'(x)\,A(x)\,e^{-sA_-^2}$, $x \in \mathbb{R}$*, are families of trace-class operators in* H *for a.e.* $x \in \mathbb{R}$ *with*

$$
\begin{aligned}
(r,s) &\mapsto \int_{\mathbb{R}} \left\| e^{-rA_-^2} A(x)\,A'(x)\,e^{-sA_-^2} \right\|_{S^1(H)} \mathrm{d}x \in I^{log}_{-1/4,-1/4},\\
(r,s) &\mapsto \int_{\mathbb{R}} \left\| e^{-rA_-^2} A'(x)\,A(x)\,e^{-sA_-^2} \right\|_{S^1(H)} \mathrm{d}x \in I^{log}_{-1/4,-1/4}.
\end{aligned}
\tag{175}
$$

Proof. Let $0 < r, s$. then for a.e. $x \in \mathbb{R}$ the family

$$
u \mapsto e^{-(r-u)A_-^2} A(x)\,e^{-uA_-^2} A'(x)\,e^{-sA_-^2}
$$

is a continuously differentiable family of trace-class operators in H for $u \in (0, r/2)$ with derivative

$$
\begin{aligned}
&\partial_u \left(e^{-(r-u)A_-^2} A(x)\,e^{-uA_-^2} A'(x)\,e^{-sA_-^2} \right)\\
=&A_-^2 e^{-(r-u)A_-^2} A(x)\,e^{-uA_-^2} A'(x)\,e^{-sA_-^2} - e^{-(r-u)A_-^2} A(x)\,A_-^2 e^{-uA_-^2} A'(x)\,e^{-sA_-^2}\\
=&A_-^2 e^{-(r-u)A_-^2} \left\{ A(x)\,e^{-u/2A_-^2} \right\} e^{-u/2A_-^2} A'(x)\,e^{-sA_-^2}\\
&- \left\{ e^{-(r-u)A_-^2} A(x)\,A_- \right\} A_- e^{-u/2A_-^2} e^{-u/2A_-^2} A'(x)\,e^{-sA_-^2},
\end{aligned}
\tag{176}
$$

where in the last step we used that $(A(x)\,A_-)^* \supseteq A_- A(x)$, $x \in \mathbb{R}$, the fact that

$$
\left\{ A_- A(x)\,e^{-(r-u)A_-^2} \right\}
$$

exists and Lemma 2.19. The derivative (176) is indeed continuous in $S^1(H)$ because the norm continuity of $e^{-tA_-^2}$ for $t > 0$ (Lemma 2.37), together with the fact that $e^{-tA_-^2} A'(x)\,e^{-vA_-^2}$ is trace-class for $t, v > 0$ and a.e. $x \in \mathbb{R}$, implies that the last expression in (176) is $S^1(H)$-continuous in $u \in (0, r/2)$. Furthermore, we may estimate the derivatives norm in $S^1(H)$ for $0, r, s \le t_0$ according to Corollary 2.39 and Lemma 2.23 by

$$
\left\| \partial_u \left(e^{-(r-u)A_-^2} A(x)\,e^{-uA_-^2} A'(x)\,e^{-sA_-^2} \right) \right\|_{S^1(H)} \lesssim_{t_0} (r-u)^{-1} u^{-1/2} g(u,s,x), \tag{177}
$$

where $g(u,s,x) := \left\| e^{-u/2A_-^2} A'(x)\,e^{-sA_-^2} \right\|_{S^1(H)}$. We note that this bound is integrable in $u \in (0, r/2)$ for a.e. $x \in \mathbb{R}$. Since the derivative (176) is continuous in $S^1(H)$, and thus

$S^1(H)$-measurable on $(0, r/2)$, we conclude that the Bochner-integral converges in $S^1(H)$ and therefore

$$\begin{aligned}
&\int_0^{r/2} \partial_u \left(e^{-(r-u)A_-^2} A(x) e^{-uA_-^2} A'(x) e^{-sA_-^2} \right) \mathrm{d}u \\
=&\left[e^{-(r-u)A_-^2} A(x) e^{-uA_-^2} A'(x) e^{-sA_-^2} \right]_{u=0}^{u=r/2} \\
=&e^{-r/2A_-^2} A(x) e^{-r/2A_-^2} A'(x) e^{-sA_-^2} - e^{-rA_-^2} A(x) A'(x) e^{-sA_-^2}
\end{aligned} \tag{178}$$

is trace-class in H for a.e. $x \in \mathbb{R}$. Let

$$f(u) := \int_0^{t_0} s^{-1/4} \log(s) \int_{\mathbb{R}} g(u, s, x) \, \mathrm{d}x \; \mathrm{d}s, \tag{179}$$

then,

$$\begin{aligned}
&\int_0^{t_0} \int_0^{t_0} r^{-1/4} s^{-1/4} \log(r) \log(s) \int_{\mathbb{R}} \Big\| e^{-r/2A_-^2} A(x) e^{-r/2A_-^2} A'(x) e^{-sA_-^2} \\
&\qquad\qquad - e^{-rA_-^2} A(x) A'(x) e^{-sA_-^2} \Big\|_{S^1(H)} \mathrm{d}x \; \mathrm{d}s \; \mathrm{d}r \\
\lesssim_{t_0} &\int_0^{t_0} r^{-1/4} \log(r) \int_0^{r/2} (r-u)^{-1} u^{-1/2} f(u) \, \mathrm{d}u \; \mathrm{d}r \\
\lesssim_{t_0} &\int_0^{t_0/2} u^{-3/4} f(u) \int_{2u}^{t_0} (r-u)^{-1} \, \mathrm{d}r \; \mathrm{d}u \lesssim_{t_0} \int_0^{t_0/2} \log(t_0/u - 1) \, u^{-3/4} f(u) \, \mathrm{d}u \\
\lesssim_{t_0} &\int_0^{t_0/2} \int_0^{t_0} u^{-3/4} (\log(t_0 - u) - \log(u)) \, s^{-1/4} \log(s) \int_{\mathbb{R}} g(u, s, x) \, \mathrm{d}x \; \mathrm{d}s \; \mathrm{d}u \\
<&\infty.
\end{aligned} \tag{180}$$

In the penultimate step we used that

$$(u, s) \mapsto \int_{\mathbb{R}} g(u, s, x) \, \mathrm{d}x \in I^{log}_{-3/4, -1/4}. \tag{181}$$

We note that

$$e^{-r/2A_-^2} A(x) e^{-r/2A_-^2} A'(x) e^{-sA_-^2}, \tag{182}$$

is trace-class in H for a.e. $x \in \mathbb{R}$, and that its trace-norm can be estimated by

$$\left\| e^{-r/2A_-^2} A(x) e^{-r/2A_-^2} A'(x) e^{-sA_-^2} \right\|_{S^1(H)} \lesssim_{t_0} r^{-1/2} g(r, s, x), \tag{183}$$

therefore we have

$$(r, s) \mapsto \int_{\mathbb{R}} \left\| e^{-r/2A_-^2} A(x) e^{-r/2A_-^2} A'(x) e^{-sA_-^2} \right\|_{S^1(H)} \mathrm{d}x \in I^{log}_{-1/4, -1/4}. \tag{184}$$

Together with our previous results (178) and (180) we conclude that for $r, s > 0$ the operator

$$e^{-rA_-^2} A(x) A'(x) e^{-sA_-^2}$$

is trace-class in H for a.e. $x \in \mathbb{R}$ and that

$$\int_{\mathbb{R}} \left\| e^{-rA_-^2} A(x) A'(x) e^{-sA_-^2} \right\|_{S^1(H)} \mathrm{d}x \in I_{-1/4,-1/4}^{log}. \tag{185}$$

For the operator

$$e^{-rA_-^2} A'(x) A(x) e^{-sA_-^2}$$

we proceed analogously, and use that

$$(r,s) \mapsto \int_{\mathbb{R}} \left\| e^{-rA_-^2} A'(x) e^{-sA_-^2} \right\|_{S^1(H)} \in I_{-1/4,-3/4}^{log}. \tag{186}$$

■

3.2 The spectral shift function of the pair (A_+, A_-)

In the previous subsection 3.1 we have shown enough trace-class memberships related to A_+ and A_-, such that we may construct their spectral shift function.

We first prove that there is a spectral shift function of the pair (A_+, A_-), uniquely determined up to a constant, by a result of Koplienko [24].
To that end, we have to discuss the resolvent comparability in trace class of A_+ and A_-

Lemma 3.5. *Define*

$$R_\pm := (A_\pm - \mathbb{i})^{-1}, \tag{187}$$

and let

$$g(s,t) := \int_{\mathbb{R}} \left\| e^{-sA_-^2} A'(x) e^{-tA_-^2} \right\|_{S^1(H)} \mathrm{d}x, \ \ s,t > 0. \tag{188}$$

- *If* $g \in I_{-1/2,-1/2}$ *then* $R_+ - R_- \in S^1(H)$.
- *If* $g \in I_{-1/2,0}$ *then* $(R_+ - R_-) R_- \in S^1(H)$ *and* $R_+ - R_- \in S^2(H)$.

Proof. We start with the first statement. Noting that R_- maps H continuously into the domains $\mathrm{Dom}(A_-)_\Gamma = \mathrm{Dom}(A_+)_\Gamma$, by the resolvent identity, we find

$$\begin{aligned} &R_+ - R_- = -R_+ (A_+ - A_-) R_- \\ &= -\left\{ R_+ \left(A_-^2 + 1\right)^{1/2} \right\} \left(A_-^2 + 1\right)^{-1/2} (A_+ - A_-) \left(A_-^2 + 1\right)^{-1/2} \left(A_-^2 + 1\right)^{1/2} R_-. \end{aligned} \tag{189}$$

Denoting the bounded operators

$$B_1 := -\left\{R_+\left(A_-^2+1\right)^{1/2}\right\},\ B_2 := \left(A_-^2+1\right)^{1/2}R_-, \tag{190}$$

we proceed to calculate

$$\begin{aligned}R_+ - R_- &= B_1\int_0^\infty\int_0^\infty e^{-s}\left(\pi s\right)^{-1/2}\left(\pi t\right)^{-1/2}e^{-t}e^{-sA_-^2}\left(A_+ - A_-\right)e^{-tA_-^2}\mathrm{d}s\ \mathrm{d}t\ B_2\\ =&\pi^{-1}B_1\int_0^\infty\int_0^\infty e^{-s}\left(st\right)^{-1/2}e^{-t}\int_{\mathbb{R}}e^{-sA_-^2}A'\left(x\right)e^{-tA_-^2}\mathrm{d}x\ \mathrm{d}s\ \mathrm{d}t\ B_2.\end{aligned} \tag{191}$$

A priori, the innermost integral and hence the whole expression (the other integrals converge strongly,) converges only in the weak operator topology, by Definition 2.3, since $A'\left(x\right)$ is a derivative in the weak operator topology. However, for $s,t>0$ the family $x\mapsto e^{-sA_-^2}A'\left(x\right)e^{-tA_-^2}$ is a family of trace-class operators in H and $g\in I_{-1/2,-1/2}$. Since g is monotonously decreasing in both $s,t>0$, together with the decay of e^{-s} and e^{-t}, we conclude that

$$\int_0^\infty\int_0^\infty e^{-s}\left(st\right)^{-1/2}e^{-t}\int_{\mathbb{R}}\left\|e^{-sA_-^2}A'\left(x\right)e^{-tA_-^2}\right\|_{S^1(H)}\mathrm{d}x\ \mathrm{d}s\ \mathrm{d}t<\infty. \tag{192}$$

Together with the fact that

$$\left(0,\infty\right)^2\times\mathbb{R}\ni\left(s,t,x\right)\mapsto\left(st\right)^{-1/2}e^{-s}e^{-t}e^{-sA_-^2}A'\left(x\right)e^{-tA_-^2}$$

is weakly measurable in $B\left(H\right)$ (by continuity), we conclude, by Lemma 2.41, that

$$\left(s,t,x\right)\mapsto\left(st\right)^{-1/2}e^{-s}e^{-t}e^{-sA_-^2}A'\left(x\right)e^{-tA_-^2}\in L^1\left(\left(0,\infty\right)^2\times\mathbb{R},S^1\left(H\right)\right). \tag{193}$$

Thus, the integral in formula (191) converges in trace-class and therefore $R_+ - R_- \in S^1\left(H\right)$.

For the second statement, in case of $g\in I_{-1/2,0}$, one concludes completely analogously that

$$\begin{aligned}\left(R_+ - R_-\right)R_- &= -R_+\left(A_+ - A_-\right)R_-^2\\ =-&\left\{R_+\left(A_-^2+1\right)^{1/2}\right\}\left(A_-^2+1\right)^{-1/2}\left(A_+ - A_-\right)\left(A_-^2+1\right)^{-1}\left(A_-^2+1\right)R_-^2.\end{aligned} \tag{194}$$

Noticing that

$$-\left\{R_+\left(A_-^2+1\right)^{1/2}\right\},\ \left(A_-^2+1\right)R_-^2,$$

are bounded operators, we proceed to calculate

$$\begin{aligned}&\left(A_-^2+1\right)^{-1/2}\left(A_+ - A_-\right)\left(A_-^2+1\right)^{-1}\\ =&\pi^{-1/2}\int_0^\infty\int_0^\infty e^{-s}s^{-1/2}e^{-t}\int_{\mathbb{R}}e^{-sA_-^2}A'\left(x\right)e^{-tA_-^2}\mathrm{d}x\ \mathrm{d}s\ \mathrm{d}t.\end{aligned} \tag{195}$$

The above integral 195 converges analogously to the integral 191 of the first statement in $S^1(H)$, because $g \in I_{-1/2,0}$, and therefore $(R_+ - R_-) R_- \in S^1(H)$. Further, we note that $R_+ - R_- \in S^2(H)$, is equivalent to $(R_+ - R_-)^* (R_+ - R_-) \in S^1(H)$. We investigate the latter expression

$$
\begin{aligned}
&(R_+ - R_-)^* (R_+ - R_-) = -R_+^* (A_+ - A_-) R_-^* R_- (A_+ - A_-) R_+ \\
=&B_3 \left(A_-^2 + 1\right)^{-1/2} (A_+ - A_-) \left(A_-^2 + 1\right)^{-1} B_4,
\end{aligned} \tag{196}
$$

where

$$
B_3 := -\left\{R_+^* \left(A_-^2 + 1\right)^{1/2}\right\}, \; B_4 := (A_+ - A_-) R_+, \tag{197}
$$

are bounded operators in H. Since

$$
\left(A_-^2 + 1\right)^{-1/2} (A_+ - A_-) \left(A_-^2 + 1\right)^{-1},
$$

is trace-class in H, by (195), we conclude that $R_+ - R_- \in S^2(H)$. ■

Proposition 3.6. *Let*

$$
g(s,t) := \int_{\mathbb{R}} \left\| e^{-sA_-^2} A'(x) e^{-tA_-^2} \right\|_{S^1(H)} \mathrm{d}x, \; s, t > 0. \tag{198}
$$

1. *If $g \in I_{-1/2,-1/2}$, then there exists a spectral shift function $\xi(\cdot, A_+, A_-)$ associated to the pair (A_+, A_-), such that*

$$
\xi(\cdot, A_+, A_-) \in L^1\left(\mathbb{R}, \left(\nu^2 + 1\right)^{-1} \mathrm{d}\nu\right). \tag{199}
$$

Additionally we have the trace formula

$$
\begin{aligned}
f(A_+) - f(A_-) &\in S^1(H), \\
\mathrm{tr}_H (f(A_+) - f(A_-)) &= \int_{\mathbb{R}} f'(\nu) \xi(\nu, A_+, A_-) \mathrm{d}\nu,
\end{aligned} \tag{200}
$$

where f is twice weakly differentiable with locally bounded derivatives and there is $\epsilon > 0$ such that

$$
\begin{aligned}
&\left(\nu^2 f'(\nu)\right)' =_{|\nu|\to\infty} O\left(|\nu|^{-1-\epsilon}\right), \\
\lim_{\nu\to-\infty} f(\nu) = \lim_{\nu\to+\infty} f(\nu), \quad &\lim_{\nu\to-\infty} \nu^2 f'(\nu) = \lim_{\nu\to+\infty} \nu^2 f'(\nu).
\end{aligned} \tag{201}
$$

2. *If $g \in I_{-1/2,0}$ (this is implied by Hypothesis A2 (2.11)), then there exists a spectral shift function $\xi(\cdot, A_+, A_-)$ associated to the pair (A_+, A_-), such that*

$$
\xi(\cdot, A_+, A_-) \in L^1\left(\mathbb{R}, \left(\nu^2 + 1\right)^{-(r/2+1)} \mathrm{d}\nu\right), \quad \textit{for all } r > 1. \tag{202}
$$

Additionally we have the trace formula

$$f(A_+) - f(A_-) \in S^1(H),$$
$$\operatorname{tr}_H (f(A_+) - f(A_-)) = \int_{\mathbb{R}} f'(\nu)\,\xi(\nu, A_+, A_-)\,\mathrm{d}\nu, \tag{203}$$

where f is twice weakly differentiable with locally bounded derivatives and there is $r > 1$ such that

$$\left(\nu^2 f'(\nu)\right)' =_{|\nu|\to\infty} O\left(|\nu|^{-1-r}\right),$$
$$\lim_{\nu\to-\infty} f(\nu) = \lim_{\nu\to+\infty} f(\nu), \quad \lim_{\nu\to\pm\infty} \nu^2 f'(\nu) = 0. \tag{204}$$

Proof. By Lemma 3.5, we have, in case of $g \in I_{-1/2,-1/2}$, that $R_+ - R_- \in S^1(H)$. Together with the conditions posed on f, the prerequisites of [38, Theorem 8.7.1] are fulfilled, thus proving the first statement.
In case of $g \in I_{-1/2,0}$, we may not use [38, Theorem 8.7.1], but instead we have to use a similar result by Koplienko, namely [24, Theorem 1.7]. We need to check that its prerequisites are satisfied. While Lemma 3.5 grants us the existence of a spectral shift function with respect to A_+ and A_-, we need to check that the conditions on f suffice to infer the trace formula (203). Let

$$\zeta = \frac{\mathbb{i} - \nu}{\mathbb{i} + \nu} \in \mathbb{T}\setminus\{-1\} \tag{205}$$

be the Cayley transform of $\nu \in \mathbb{R}$ to $\zeta \in \mathbb{T}$, $\mathbb{T}$ denoting the 1-dimensional torus. Let $h(\zeta) := f(\nu)$. We note that

$$-2\mathbb{i}h'(\zeta) = (\mathbb{i} + \nu)^2 f'(\nu),$$
$$-4h''(\zeta) = (\mathbb{i} - \nu)^2 \left((\mathbb{i} + \nu)^2 f'(\nu)\right)'. \tag{206}$$

Therefore, the conditions on f imply that g is twice differentiable on $\mathbb{T}$ (and thus g' is Hölder-continuous) and that, by the mean value theorem, we have

$$h'(\zeta) = O(|\zeta + 1|^r), \quad \text{for } \zeta \to -1. \tag{207}$$

Therefore, $h \in \Phi_r(-1)$, which in turn means that $f \in Y_r$, where Φ_r and Y_r are defined in [24]. Thus, [24, Theorem 1.7] can be applied and f is amenable for the trace formula (203). ■

In contrast to Proposition 3.6, we may define the spectral shift function η of the pair (A_+, A_-) according to equation [38, (8.11.4)], if $0 \in \rho(A_+) \cap \rho(A_-)$. We therefore need the trace comparability of the inverses of A_+ and A_-.

Lemma 3.7. *Let $0 \in \rho(A_+) \cap \rho(A_-)$. Let*

$$(s,t) \mapsto g(s,t) := \int_{\mathbb{R}} \left\| e^{-sA_-^2} A'(x)\, e^{-tA_-^2} \right\|_{S^1(H)} \mathrm{d}x \in I_{-1/2,-1/2}. \tag{208}$$

Then $A_+^{-1} - A_-^{-1} \in S^1(H)$.

Proof. The proof of this Proposition is largely analogous to the proof of Lemma 3.5. We start with the resolvent identity and use the invertibility of A_- and A_+ to conclude that

$$\begin{aligned} A_+^{-1} - A_-^{-1} &= -A_+^{-1}\left(A_+ - A_-\right)A_-^{-1} \\ &= \left\{A_+^{-1}\left(A_-^2+1\right)^{1/2}\right\}\left(A_-^2+1\right)^{-1/2}\left(A_+ - A_-\right)\left(A_-^2+1\right)^{-1/2}\left(A_-^2+1\right)^{1/2}A_-^{-1}. \end{aligned} \tag{209}$$

Since

$$\left(A_-^2+1\right)^{-1/2}\left(A_+ - A_-\right)\left(A_-^2+1\right)^{-1/2},$$

is trace-class in H, as shown in the proof of Lemma 3.5, we finish the proof by noting that

$$\left\{A_+^{-1}\left(A_-^2+1\right)^{1/2}\right\},\ \left(A_-^2+1\right)^{1/2}A_-^{-1},$$

are bounded operators in H. ■

Definition 3.8. Let $0 \in \rho(A_+) \cap \rho(A_-)$ and

$$(s,t) \mapsto g(s,t) := \int_{\mathbb{R}} \left\| e^{-sA_-^2} A'(x)\, e^{-tA_-^2} \right\|_{S^1(H)} \mathrm{d}x \in I_{-1/2,-1/2}. \tag{210}$$

Then define the spectral shift function η of the pair (A_+, A_-) by

$$\begin{aligned} &\eta(\mu, A_+, A_-) := -\xi\left(\mu^{-1}, A_+^{-1}, A_-^{-1}\right), \quad \text{for } \mu \neq 0, \\ &\eta(0, A_+, A_-) := 0. \end{aligned} \tag{211}$$

Here $\xi\left(\cdot, A_+^{-1}, A_-^{-1}\right)$ is the spectral shift function of the pair $\left(A_+^{-1}, A_-^{-1}\right)$ defined according to [38, Theorem 8.2.1], i.e.

$$\xi\left(\mu, A_+^{-1}, A_-^{-1}\right) := \pi^{-1} \lim_{\epsilon \searrow 0} \Im\left(\log\left(\det{}_H\left(1 + \left(A_+^{-1} - A_-^{-1}\right)\left(A_-^{-1} - \mu - i\epsilon\right)^{-1}\right)\right)\right), \tag{212}$$

where the branches of $\log\det{}_H$ in the upper and lower half-plane are chosen such that

$$\lim_{|\Im(z)| \to \infty} \log\left(\det{}_H\left(1 + \left(A_+^{-1} - A_-^{-1}\right)\left(A_-^{-1} - z\right)^{-1}\right)\right) = 0. \tag{213}$$

Let us summarize some of the properties of the spectral shift function $\eta(\cdot, A_+, A_-)$.

Proposition 3.9. *The spectral shift function $\eta(\cdot, A_+, A_-)$ from Definition 3.8 is well-defined. $\eta(\cdot, A_+, A_-)$ is constantly 0 in a neighbourhood of 0, and*

$$\eta(\cdot, A_+, A_-) \in L^1\left(\mathbb{R}, \left(\mu^2+1\right)^{-1}\mathrm{d}\mu\right). \tag{214}$$

Also the trace formula

$$\begin{aligned} &f(A_+) - f(A_-) \in S^1(H), \\ &\mathrm{tr}_H\left(f(A_+) - f(A_-)\right) = \int_{\mathbb{R}} f'(\mu)\, \eta(\mu, A_+, A_-)\, \mathrm{d}\mu, \end{aligned} \tag{215}$$

holds for functions f, which are twice differentiable, with locally bounded second derivative and that for some $\delta > 0$, we have

$$\left|\left(\mu^2 f'(\mu)\right)'\right| \lesssim_\delta |\mu|^{-1-\delta}, \quad \textit{for } \mu \in \mathbb{R},$$
$$\lim_{\mu\to-\infty} f(\mu) = \lim_{\mu\to+\infty} f(\mu), \quad \lim_{\mu\to-\infty} \mu^2 f'(\mu) = \lim_{\mu\to+\infty} \mu^2 f'(\mu). \tag{216}$$

Proof. Since $0 \in \rho(A_+) \cap \rho(A_-)$, there exists $\epsilon > 0$ such that $(-2\epsilon, 2\epsilon) \subset \rho(A_+) \cap \rho(A_-)$. Consider the intervals $\Omega_1 = (-\infty, -\epsilon)$ and $\Omega_2 = (\epsilon, \infty)$. Clearly the spectra of A_+ and A_- are covered by $\Omega = \Omega_1 \cup \Omega_2$. Let $\phi(\mu) := \mu^{-1}$. Then

$$\phi'(\mu) = -\mu^{-2} < 0, \quad \text{for } \mu \in \Omega. \tag{217}$$

Since additionally ϕ is one-to-one, bounded, and twice continuously differentiable on Ω, we conclude that ϕ and the covering Ω_1, Ω_2 satisfy [38, Condition 2, §11]. Therefore, by equation [38, (8.11.4)] and Lemma 3.7, we may define the spectral shift function η of (A_+, A_-) by

$$\eta(\mu, A_+, A_-) = -\xi\left(\mu^{-1}, A_+^{-1}, A_-^{-1}\right), \quad \text{for } \mu \in \Omega. \tag{218}$$

It remains to determine η on $\mathbb{R}\backslash\Omega$. The function $\xi\left(\cdot, A_+^{-1}, A_-^{-1}\right)$ is defined on all of $\mathbb{R}$ by [38, Theorem 8.2.1] and $\xi\left(\cdot, A_+^{-1}, A_-^{-1}\right) \in L^1(\mathbb{R})$. Furthermore, since

$$\mathbb{R}\backslash\left(-(2\epsilon)^{-1}, (2\epsilon)^{-1}\right) \subset \rho\left(A_+^{-1}\right) \cap \rho\left(A_-^{-1}\right), \tag{219}$$

we may conclude by [38, Proposition 8.2.8], that $\xi\left(\cdot, A_+^{-1}, A_-^{-1}\right)$ is constant on $\mathbb{R}\backslash\left(-(2\epsilon)^{-1}, (2\epsilon)^{-1}\right)$. Together with the integrability of $\xi\left(\cdot, A_+^{-1}, A_-^{-1}\right)$, we conclude that this constant must be 0. Therefore Definition 3.8 is well-defined, and furthermore $\eta(\cdot, A_+, A_-)$ is identically 0 in a neighbourhood of 0. According to [38, Theorem 8.11.5] the trace formula,

$$f(A_+) - f(A_-) \in S^1(H),$$
$$\operatorname{tr}_H\left(f(A_+) - f(A_-)\right) = \int_{\mathbb{R}} f'(\mu)\,\eta(\mu, A_+, A_-)\,\mathrm{d}\mu, \tag{220}$$

holds for functions f, which are twice differentiable, with locally bounded second derivative and that for some $\delta > 0$ we have

$$\left|\left(\mu^2 f'(\mu)\right)'\right| \lesssim_\delta |\mu|^{-1-\delta}, \quad \text{for } \mu \in \Omega,$$
$$\lim_{\mu\to-\infty} f(\mu) = \lim_{\mu\to+\infty} f(\mu), \quad \lim_{\mu\to-\infty} \mu^2 f'(\mu) = \lim_{\mu\to+\infty} \mu^2 f'(\mu). \tag{221}$$

Additionally, following inequality [38, (8.2.6)] and the transformation rule, we find

$$\int_{\mathbb{R}} |\eta(\mu, A_+, A_-)|\left(\mu^2+1\right)^{-1} \mathrm{d}\mu \lesssim \int_{\Omega} |\eta(\mu, A_+, A_-)|\left|\phi'(\mu)\right| \mathrm{d}\mu \lesssim \left\|A_+^{-1} - A_-^{-1}\right\|_{S^1(H)}$$
$$<\infty. \tag{222}$$

■

3.3 Operators in $S^1\left(L^2(\mathbb{R},H)\right)$

In this subsection we develop the necessary statements on trace-class memberships of operators in $L^2(\mathbb{R},H)$, especially those in connection with the left hand side of the trace formulae (1). To do so we need a tool for "lifting" a trace class operator family in H to a trace class operator in $L^2(\mathbb{R},H)$. It relies on the well known fact that Hilbert-Schmidt operators are tensorial, which is for example presented in [16, Lemma 4.5].

Lemma 3.10. *Let X be a complex, separable Hilbert space. Suppose $t(x,y)\in S^2(X)$ for a.e. $(x,y)\in\mathbb{R}^2$ and assume that*

$$\int_{\mathbb{R}^2}\|t(x,y)\|^2_{S^2(X)}\,\mathrm{d}y\ \mathrm{d}x<\infty. \tag{223}$$

Define the integral operator T in $L^2(\mathbb{R},X)$ by

$$(Tf)(x):=\int_{\mathbb{R}}t(x,y)\,f(y)\,\mathrm{d}y \text{ for a.e. } x\in\mathbb{R},\quad f\in L^2(\mathbb{R},H). \tag{224}$$

Then $T\in S^2\left(L^2(\mathbb{R},X)\right)$, and

$$\|T\|^2_{S^2(L^2(\mathbb{R},H))}=\int_{\mathbb{R}^2}\|t(x,y)\|^2_{S^2(X)}\,\mathrm{d}y\ \mathrm{d}x. \tag{225}$$

Conversely, any operator $T\in S^2\left(L^2(\mathbb{R},X)\right)$ arises in the manner (223), (224).

Remark 3.11. Lemma 3.10 is, of course, the concrete isometric isomorphism in the tensorial identification $L^2\left(\mathbb{R}^2\right)\widehat{\otimes}S^2(X)\cong S^2\left(L^2(\mathbb{R},X)\right)\cong S^2\left(L^2(\mathbb{R})\widehat{\otimes}X\right)$.

We use the above property of the Hilbert-Schmidt operators for Proposition 3.12 below, by splitting the operator therein into to Hilbert-Schmidt operators. The conditions on the auxiliary operators K_1,K_2 resemble the conditions on the auxiliary functions in the famous Schur test (c.f. [18, Theorem 5.2]), from which we therefore borrowed the name.

Proposition 3.12. *Assume K_1,K_2 are integral kernel operators in $L^2(\mathbb{R})$ given by $\mathbb{R}^2$-measurable functions k_1,k_2, satisfying a Schur test condition, i.e.*

$$(K_if)(x)=\int_{\mathbb{R}}k_i(x,y)\,f(y)\,\mathrm{d}y,\ \text{for a.e. } x\in\mathbb{R},\quad f\in L^2(\mathbb{R}),$$

$$\sup_{y\in\mathbb{R}}\int_{\mathbb{R}}|k_1(x,y)|^2\,\mathrm{d}x<\infty \text{ and } \sup_{x\in\mathbb{R}}\int_{\mathbb{R}}|k_2(x,y)|^2\,\mathrm{d}y<\infty. \tag{226}$$

Assume further that $B(\cdot)\in L^1\left(\mathbb{R},S^1(H)\right)$ (c.f. Lemma 2.41).
Define the operator T in $L^2(\mathbb{R},H)$ by

$$T:=K_1^HB(X)\,K_2^H, \tag{227}$$

where $K_i^H:=K_i\widehat{\otimes}1_H\in B\left(L^2(\mathbb{R},H)\right)$ for $i\in\{1,2\}$. Then $T\in S^1\left(L^2(\mathbb{R},H)\right)$ and

$$\|T\|_{S^1(L^2(\mathbb{R},H))}\leq\left(\sup_{y\in\mathbb{R}}\int_{\mathbb{R}}|k_1(x,y)|^2\,\mathrm{d}x\right)^{1/2}\Big\|\|B(\cdot)\|_{S^1(H)}\Big\|_{L^1(\mathbb{R})}\left(\sup_{x\in\mathbb{R}}\int_{\mathbb{R}}|k_2(x,y)|^2\,\mathrm{d}y\right)^{1/2}. \tag{228}$$

Proof. Let $(e_n)_{n\in\mathbb{N}}$ be a orthonormal basis of H. For a.e. $x \in \mathbb{R}$ we have a polar decomposition $B(x) = U(x)|B(x)|$, where $U(x)$ is an isometry of H and $|B(x)| = (B(x)^* B(x))^{1/2}$. Let $T_1(x) := U(x)|B(x)|^{1/2}$ and $T_2(x) := |B(x)|^{1/2}$. Then

$$\begin{aligned}\|T_1(x)\|^2_{S^2(H)} &= \sum_{n\in\mathbb{N}} \left\|U(x)|B(x)|^{1/2} e_n\right\|_H = \sum_{n\in\mathbb{N}} \left\||B(x)|^{1/2} e_n\right\|_H = \|T_2(x)\|^2_{S^2(H)} \\ &= \sum_{n\in\mathbb{N}} \langle |B(x)| e_n, e_n\rangle_H = \|B(x)\|_{S^1(H)}. \end{aligned} \tag{229}$$

The operators $T_i(X)$ and $B(X)$ are not necessarily bounded operators in $L^2(\mathbb{R}, H)$. However, they are densely defined since (essentially) bounded $L^2(\mathbb{R}, H)$ functions are contained in their domains. Therefore, by the Schur test condition (226), K_2^H maps into the domains of $T_2(X)$ and $B(X)$ and furthermore $T_2(X) K_2^H$ and T are bounded. Since K_1^* has the same Schur test condition as K_2 and $T_1(X)^*$ is bounded on the (essentially) bounded $L^2(\mathbb{R}, H)$ functions, the bounded operator $\left\{T_1(X)^* \left(K_1^H\right)^*\right\}$ exists. Additionally T_1 is closed by Lemma 2.44. Lemma 2.19 then implies that also $\left\{K_1^H T_1(X)\right\}$ exists. We furthermore have

$$\begin{aligned}\left(\left\{K_1^H T_1(X)\right\} g\right)(x) &= \int_{\mathbb{R}} k_1(x,y)\cdot(T_1(y) g(y))\,\mathrm{d}y, \text{ for a.e. } x\in\mathbb{R}, \quad g\in L^2(\mathbb{R},H), \\ \left(T_2(X) K_2^H g\right)(x) &= \int_{\mathbb{R}} k_2(x,y)\cdot(T_2(x) g(y))\,\mathrm{d}y, \text{ for a.e. } x\in\mathbb{R}, \quad g\in L^2(\mathbb{R},H).\end{aligned} \tag{230}$$

For the Hilbert-Schmidt norm we estimate by Lemma 3.10 , equation (229) and the Schur test condition (226):

$$\begin{aligned}\left\|\left\{K_1^H T_1(X)\right\}\right\|^2_{S^2(L^2(\mathbb{R},H))} &= \int_{\mathbb{R}^2} |k_1(x,y)|^2 \cdot \|T_1(y)\|^2_{S^2(H)}\,\mathrm{d}y\ \mathrm{d}x \\ &= \int_{\mathbb{R}^2} |k_1(x,y)|^2 \cdot \|B(y)\|_{S^1(H)}\,\mathrm{d}y\ \mathrm{d}x \\ &\le \sup_{y\in\mathbb{R}} \int_{\mathbb{R}} |k_1(x,y)|^2\,\mathrm{d}x \cdot \left\|\|B(\cdot)\|_{S^1(H)}\right\|_{L^1(\mathbb{R})} < \infty. \\ \left\|T_2(X) K_2^H\right\|^2_{S^2(L^2(\mathbb{R},H))} &= \int_{\mathbb{R}^2} |k_2(x,y)|^2 \cdot \|T_2(x)\|^2_{S^2(H)}\,\mathrm{d}y\ \mathrm{d}x \\ &= \int_{\mathbb{R}^2} |k_2(x,y)|^2 \cdot \|B(x)\|_{S^1(H)}\,\mathrm{d}y\ \mathrm{d}x \\ &\le \sup_{x\in\mathbb{R}} \int_{\mathbb{R}} |k_2(x,y)|^2\,\mathrm{d}y \cdot \left\|\|B(\cdot)\|_{S^1(H)}\right\|_{L^1(\mathbb{R})} < \infty. \end{aligned} \tag{231}$$

Thus $K_1^H T_1(X) T_2(X) K_2^H = T$ is trace-class in $L^2(\mathbb{R}, H)$ and

$$\begin{aligned}&\|T\|_{S^1(L^2(\mathbb{R},H))} \le \left\|\left\{K_1^H T_1(X)\right\}\right\|_{S^2(L^2(\mathbb{R},H))} \cdot \left\|T_2(X) K_2^H\right\|_{S^2(L^2(\mathbb{R},H))} \\ &\le \left(\sup_{y\in\mathbb{R}} \int_{\mathbb{R}} |k_1(x,y)|^2\,\mathrm{d}x\right)^{1/2} \left\|\|B(\cdot)\|_{S^1(H)}\right\|_{L^1(\mathbb{R})} \left(\sup_{x\in\mathbb{R}} \int_{\mathbb{R}} |k_2(x,y)|^2\,\mathrm{d}y\right)^{1/2}. \end{aligned} \tag{232}$$

■

With this tool, we can directly deduce the following trace-class memberships by using the trace-class memberships of the operator families in H presented in subsection 3.1.

Lemma 3.13. *Assume Hypothesis A2 (*2.11*) and let $B \in \{AA', A'A\}$. Then for $r, s > 0$*

$$\begin{aligned} e^{-rH_0} B(X) e^{-sH_0} &\in S^1\left(L^2(\mathbb{R}, H)\right), \\ \left((u,v) \mapsto \left\|e^{-uH_0} B(X) e^{-vH_0}\right\|_{S^1(L^2(\mathbb{R},H))}\right) &\in I^{log}_{0,0}. \end{aligned} \tag{233}$$

and

$$\begin{aligned} e^{-rH_0} A'(X) e^{-sH_0} &\in S^1\left(L^2(\mathbb{R}, H)\right), \\ \left((u,v) \mapsto \left\|e^{-uH_0} A'(X) e^{-vH_0}\right\|_{S^1(L^2(\mathbb{R},H))}\right) &\in I^{log}_{-1/2,0} \cap I^{log}_{0,-1/2}. \end{aligned} \tag{234}$$

*Assume Hypothesis A1 (*2.10*). Then for $r, s > 0$*

$$\begin{aligned} e^{-rH_0} A'(X) e^{-sH_0} &\in S^1\left(L^2(\mathbb{R}, H)\right), \\ \left((u,v) \mapsto \left\|e^{-uH_0} A'(X) e^{-vH_0}\right\|_{S^1(L^2(\mathbb{R},H))}\right) &\in I^{log}_{0,0}. \end{aligned} \tag{235}$$

Proof. Let $r, s > 0$ and $B \in \{A', AA', A'A\}$. By Lemma 2.8 and the (resolvent) commutativity of ∂ and $\widehat{A_-}$ we conclude for $t > 0$:

$$e^{-tH_0} = e^{t\partial^2} e^{-t\widehat{A_-^2}} = e^{t\partial^2_{\mathbb{C}}} \hat{\otimes} e^{-tA_-^2}. \tag{236}$$

Therefore we have

$$e^{-rH_0} B(X) e^{-sH_0} = K_1^H C_{r,s}(X) K_2^H, \tag{237}$$

where $K_1 = e^{r\partial^2_{\mathbb{C}}}$, $K_2 = e^{s\partial^2_{\mathbb{C}}}$ and $C_{r,s}(x) := e^{-rA_-^2} B(x) e^{-sA_-^2}$ for a.e. $x \in \mathbb{R}$. We want to apply Proposition 3.12 to equation (237).
For $r, s > 0$ the operator $C_{r,s}(\cdot) \in L^1\left(\mathbb{R}, S^1(H)\right)$ (for $B = A'$ directly by Hypothesis A1 (2.10) or A2 (2.11); for $B = AA'$ and $B = A'A$ by Lemma 3.4).
Furthermore we conclude by Lemma 2.36 for $t > 0$

$$\begin{aligned} &\sup_{x \in \mathbb{R}} \int_{\mathbb{R}} |q_t(x-y)|^2 \,\mathrm{d}y = \|q_t\|^2_{L^2(\mathbb{R})} = \sup_{y \in \mathbb{R}} \int_{\mathbb{R}} |q_t(x-y)|^2 \,\mathrm{d}x \\ &= (8\pi t)^{-1/2} < \infty. \end{aligned} \tag{238}$$

Therefore by Proposition 3.12 the operator $e^{-rH_0} B(X) e^{-sH_0}$ is trace-class in $L^2(\mathbb{R}, H)$ and

$$\left\|e^{-rH_0} B(X) e^{-sH_0}\right\|_{S^1(L^2(\mathbb{R},H))} \le (8\pi)^{-1/2} \int_{\mathbb{R}} \|C_{r,s}(x)\|_{S^1(H)} \,\mathrm{d}x \,(rs)^{-1/4} < \infty. \tag{239}$$

Furthermore we have by Hypothesis A2 (2.11) and Lemma 3.4,

$$\begin{aligned}&\left((u,v)\mapsto\|C_{u,v}(\cdot)\|_{S^1(H)}\right)\in I^{log}_{-1/4,-1/4},\ \text{for } B\in\left\{AA',A'A\right\},\\&\left((u,v)\mapsto\|C_{u,v}(\cdot)\|_{S^1(H)}\right)\in I^{log}_{-3/4,-1/4}\cap I^{log}_{-1/4,-3/4},\ \text{for } B=A',\end{aligned}\tag{240}$$

while if only Hypothesis A1 (2.10) holds we have

$$\left((u,v)\mapsto\|C_{u,v}(\cdot)\|_{S^1(H)}\right)\in I^{log}_{-1/4,-1/4},\ \text{for } B=A'.\tag{241}$$

Combining the memberships (240) and (241) with inequality (239), we obtain the claimed memberships (233), (234) and (235). ■

We use the Laplace transform similarly to Lemma 3.3, and thus may analogously prove the following Corollary 3.14.

Corollary 3.14. *Assume Hypothesis A1 (*2.10*). Then*

$$(1+H_0)^{-1}A'(X)(1+H_0)^{-1}$$

is a trace-class operator in $L^2(\mathbb{R},H)$*.*

Proof. For $f\in L^2(\mathbb{R},H)$ we have by the functional calculus

$$(1+H_0)^{-1}f=\int_0^\infty e^{-t}e^{-tH_0}f\mathrm{d}t,\tag{242}$$

where the integral converges in $L^2(\mathbb{R},H)$. Therefore we have

$$(1+H_0)^{-1}A'(X)(1+H_0)^{-1}=\int_0^\infty\int_0^\infty e^{-s}e^{-t}e^{-sH_0}A'(X)e^{-tH_0}\mathrm{d}t\ \mathrm{d}s,\tag{243}$$

where the integrals converge in the strong operator topology. However, by Lemma 3.13, the integrand of (243) is a family of trace-class operators in $L^2(\mathbb{R},H)$, which is trace-norm continuous in $(s,t)\in(0,\infty)^2$ and therefore $S^1\left(L^2(\mathbb{R},H)\right)$-measurable.
Similar to the estimate (174) in the proof of Lemma 3.3, we may show, using Lemma 3.13, that the trace norm of the integrand of (243) is integrable on $(s,t)\in(0,\infty)^2$.
Therefore, by Lemma 2.41, the integral in (243) converges in $S^1\left(L^2(\mathbb{R},H)\right)$, and hence the right hand side of (243) must be trace-class in $L^2(\mathbb{R},H)$. ■

In $L^2(\mathbb{R},H)$ we have the operator ∂, which is not given by fibre-wise multiplication in H, which is essential for the use of Proposition 3.12. However, we may use that ∂ commutes with H_0 to derive the following trace-class memberships involving ∂.

Lemma 3.15. *Assume Hypothesis A2 (*2.11*). Then for* $r,s>0$

$$\begin{aligned}&\left\{e^{-rH_0}\partial\right\}A'(X)e^{-sH_0}\in S^1\left(L^2(\mathbb{R},H)\right),\\&\left((u,v)\mapsto\left\|\left\{e^{-uH_0}\partial\right\}A'(X)e^{-vH_0}\right\|_{S^1(L^2(\mathbb{R},H))}\right)\in I^{log}_{0,0},\end{aligned}\tag{244}$$

$$\begin{aligned}&\left\{e^{-rH_0}A'(X)\right\}\partial e^{-sH_0}\in S^1\left(L^2(\mathbb{R},H)\right),\\&\left((u,v)\mapsto\left\|\left\{e^{-uH_0}A'(X)\right\}\partial e^{-vH_0}\right\|_{S^1(L^2(\mathbb{R},H))}\right)\in I^{log}_{0,0}.\end{aligned}\tag{245}$$

Proof. Let us consider only $\left\{e^{-rH_0}\partial\right\}A'(X)\,e^{-sH_0}$, for the other case is analogously proven, because

$$\left\{e^{-rH_0}A'(X)\right\}\partial e^{-sH_0}=e^{-rH_0}A'(X)\,e^{-s/2H_0}\left\{e^{-s/2H_0}\partial\right\},\tag{246}$$

by the (resolvent) commutativity of H_0 and ∂. For $r,s>0$ we have

$$\left\{e^{-rH_0}\partial\right\}A'(X)\,e^{-sH_0}=\partial e^{-r/2H_0}e^{-r/2H_0}A'(X)\,e^{-sH_0}.\tag{247}$$

Thus for all $t_0\geq r,s>0$ we have by Corollary 2.39:

$$\left\|\left\{e^{-rH_0}\partial\right\}A'(X)\,e^{-sH_0}\right\|_{S^1(L^2(\mathbb{R},H))}\lesssim_{t_0}r^{-1/2}\left\|e^{-r/2H_0}A'(X)\,e^{-sH_0}\right\|_{S^1(L^2(\mathbb{R},H))}.\tag{248}$$

Consequently, by Lemma 3.13

$$\begin{aligned}\left\{e^{-rH_0}\partial\right\}A'(X)\,e^{-sH_0}&\in S^1\left(L^2(\mathbb{R},H)\right),\\ \left((u,v)\mapsto\left\|\left\{e^{-uH_0}\partial\right\}A'(X)\,e^{-vH_0}\right\|_{S^1(L^2(\mathbb{R},H))}\right)&\in I^{log}_{0,0}.\end{aligned}\tag{249}$$

■

So far, we have only considered semi-groups of the operator H_0. To arrive at expressions involving the semi-groups of $H_\pm$, we use Duhamel's formula from Lemma 2.29. This results in the presence of a logarithmic term, which justifies that the Hypotheses A1 (2.10) and A2 (2.11) require the memberships in $I^{log}_{a,b}$ and not just $I_{a,b}$.

Lemma 3.16. *Assume Hypothesis A1 (*2.10*) and either Hypothesis B1 (*2.12*) or Hypothesis B2 (*2.14*). Then for $\epsilon_1,\epsilon_2\in\{+,-\}$ and $r,s>0$ the operator $e^{-rH_{\epsilon_1}}A'(X)\,e^{-sH_{\epsilon_2}}$ is trace-class in $L^2(\mathbb{R},H)$ and*

$$\left((u,v)\mapsto\left\|e^{-uH_{\epsilon_1}}A'(X)\,e^{-vH_{\epsilon_2}}\right\|_{S^1(L^2(\mathbb{R},H))}\right)\in I_{0,0}.\tag{250}$$

*If also Hypothesis A2 (*2.11*) holds, we have additionally*

$$\left((u,v)\mapsto\left\|e^{-uH_{\epsilon_1}}A'(X)\,e^{-vH_{\epsilon_2}}\right\|_{S^1(L^2(\mathbb{R},H))}\right)\in I_{-1/2,0}\cap I_{0,-1/2}.\tag{251}$$

Proof. Let $0<r,s\leq t_0$. We may write, using Lemma 2.29 twice,

$$\begin{aligned}&e^{-rH_{\epsilon_1}}A'(X)\,e^{-sH_{\epsilon_2}}=S_1+S_2+S_3+S_4,\\ &S_1:=e^{-r/2H_{\epsilon_1}}e^{-r/2H_0}A'(X)\,e^{-s/2H_0}e^{-s/2H_{\epsilon_2}},\\ &S_2:=-\int_0^{r/2}e^{-(r-u)H_{\epsilon_1}}M_{\epsilon_1}e^{-uH_0}A'(X)\,e^{-s/2H_0}e^{-s/2H_{\epsilon_2}}\mathrm{d}u\\ &S_3:=-\int_0^{s/2}e^{-r/2H_{\epsilon_1}}e^{-r/2H_0}A'(X)\,e^{-vH_0}M_{\epsilon_2}e^{-(s-v)H_{\epsilon_2}}\mathrm{d}v\\ &S_4:=\int_0^{r/2}\int_0^{s/2}e^{-(r-u)H_{\epsilon_1}}M_{\epsilon_1}e^{-uH_0}A'(X)\,e^{-vH_0}M_{\epsilon_2}e^{-(s-v)H_{\epsilon_2}}\mathrm{d}v\,\mathrm{d}u,\end{aligned}\tag{252}$$

where all integrals converge in $B\left(L^2\left(\mathbb{R},H\right)\right)$-norm. We note that S_1 and the integrands of $S_2,\ S_3$ and S_4 in (252) are trace-class in $L^2\left(\mathbb{R},H\right)$ and that the integrands are continuous in trace norm, by Lemma 2.37 and Lemma 3.13, and therefore are $S^1\left(L^2\left(\mathbb{R},H\right)\right)$-measurable. Let

$$g\left(u,v\right):=\left\|e^{-uH_0}A'\left(X\right)e^{-vH_0}\right\|_{S_1(L^2(\mathbb{R},H))},\ u,v>0. \tag{253}$$

By Proposition 2.28 and Lemma 2.19, the trace norm of the integrands can be bounded in the following way for $0<r,s\leq t_0$.

$$\begin{aligned}
&\left\|e^{-(r-u)H_{\pm 1}}M_{\epsilon_1}e^{-uH_0}A'\left(X\right)e^{-s/2H_0}e^{-s/2H_{\epsilon_2}}\right\|_{S^1(L^2(\mathbb{R},H))}\\
\lesssim_{t_0}&\left(r-u\right)^{-1}g\left(u,s/2\right),\\
&\left\|e^{-r/2H_{\epsilon_1}}e^{-r/2H_0}A'\left(X\right)e^{-vH_0}M_{\epsilon_2}e^{-(s-v)H_{\epsilon_2}}\right\|_{S^1(L^2(\mathbb{R},H))}\\
\lesssim_{t_0}&g\left(r/2,v\right)\left(s-v\right)^{-1}, &(254)\\
&\left\|e^{-(r-u)H_{\epsilon_1}}M_{\epsilon_1}e^{-uH_0}A'\left(X\right)e^{-vH_0}M_{\epsilon_2}e^{-(s-v)H_{\epsilon_2}}\right\|_{S^1(L^2(\mathbb{R},H))}\\
\lesssim_{t_0}&\left(r-u\right)^{-1}g\left(u,v\right)\left(s-v\right)^{-1}. &(255)
\end{aligned}$$

We note that all of these expressions (254) are integrable on $(0,r/2)$, $(0,s/2)$, and $(0,r/2)\times(0,s/2)$ respectively. Thus all operators $S_i,\ i=2,3,4$, are trace-class in $L^2\left(\mathbb{R},H\right)$ and therefore the operator $e^{-rH_{\epsilon_1}}A'\left(X\right)e^{-sH_{\epsilon_2}}$ is trace-class by Lemma 2.41 as well. Assuming Hypothesis A2 (2.11), for $\alpha=0$ or $\alpha=1/2$, we have the following trace-norm estimate of S_4

$$\begin{aligned}
&\int_0^{t_0}\int_0^{t_0}r^{-\alpha}s^{\alpha-1/2}\left\|S_4\right\|_{S^1(L^2(\mathbb{R},H))}\,\mathrm{d}s\ \mathrm{d}r\\
\lesssim_{t_0}&\int_0^{t_0}\int_0^{t_0}r^{-\alpha}s^{\alpha-1/2}\int_0^{r/2}\int_0^{s/2}\left(r-u\right)^{-1}g\left(u,v\right)\left(s-v\right)^{-1}\mathrm{d}v\ \mathrm{d}u\ \mathrm{d}s\ \mathrm{d}r\\
\lesssim_{t_0}&\int_0^{t_0/2}\int_0^{t_0/2}\left(2u\right)^{-\alpha}g\left(u,v\right)\left(2v\right)^{\alpha-1/2}\int_{2u}^{t_0}\int_{2v}^{t_0}\left(r-u\right)^{-1}\left(s-v\right)^{-1}\mathrm{d}s\ \mathrm{d}r\ \mathrm{d}v\ \mathrm{d}u\\
\lesssim_{t_0}&\int_0^{t_0/2}\int_0^{t_0/2}u^{-\alpha}\log\left(t_0/u-1\right)g\left(u,v\right)v^{\alpha-1/2}\log\left(t_0/v-1\right)\mathrm{d}v\ \mathrm{d}u<\infty, &(256)
\end{aligned}$$

since $g\in I^{log}_{-1/2,0}\cap I^{log}_{0,-1/2}$, by Lemma 3.13, and $g\left(u,v\right)$ is monotonously decreasing if u or v increase. Similarly one shows for $i=1,2,3$ that

$$\int_0^{t_0}\int_0^{t_0}r^{-\alpha}s^{\alpha-1/2}\left\|S_i\right\|_{S^1(L^2(\mathbb{R},H))}\,\mathrm{d}s\ \mathrm{d}r<\infty. \tag{257}$$

Summarily we have that

$$\left\|e^{-rH_{\epsilon_1}}A'\left(X\right)e^{-sH_{\epsilon_2}}\right\|_{S^1(L^2(\mathbb{R},H))}\in I_{-1/2,0}\cap I_{0,-1/2}. \tag{258}$$

Assuming only Hypothesis A1 (2.10), we analogously find

$$\left\| e^{-rH_{\epsilon_1}} A'(X)\, e^{-sH_{\epsilon_2}} \right\|_{S^1(L^2(\mathbb{R},H))} \in I_{0,0}. \tag{259}$$

■

Similarly, we may also use Duhamel's formula to show the trace-class memberships of the operators in the following Lemma 3.17, which are essentially build by replacing the operator $A'(X)$.

Lemma 3.17. *Assume Hypothesis A2 (*2.11*) and either Hypothesis B1 (*2.12*) or Hypothesis B2 (*2.14*). Let $B := AA' + A'A$. Then for $\epsilon_1, \epsilon_2 \in \{+,-\}$ and $r, s > 0$ the operators*

$$\begin{aligned} T_1(r,s) &= e^{-rH_{\epsilon_1}} B(X)\, e^{-sH_{\epsilon_2}}, \\ T_2(r,s) &= \left\{ e^{-rH_{\epsilon_1}} A'(X) \right\} \partial e^{-sH_{\epsilon_2}} \text{ and} \\ T_3(r,s) &= \left\{ e^{-rH_{\epsilon_1}} \partial \right\} A'(X)\, e^{-sH_{\epsilon_2}}, \end{aligned} \tag{260}$$

are trace-class in $L^2(\mathbb{R}, H)$ and for $i \in \{1,2,3\}$

$$\Big((u,v) \mapsto \| T_i(u,v) \|_{S^1(L^2(\mathbb{R},H))} \Big) \in I_{0,0}. \tag{261}$$

Proof. The proof of this Lemma is very similar to that of Lemma 3.16. We will therefore only point out the essential steps which differ. For T_1 there are no important differences, one replaces $A'(X)$ with $B(X)$, obtaining

$$\begin{aligned} & e^{-rH_{\epsilon_1}} B(X)\, e^{-sH_{\epsilon_2}} = S_1 + S_2 + S_3 + S_4, \\ & S_1 := e^{-r/2H_{\epsilon_1}} e^{-r/2H_0} B(X)\, e^{-s/2H_0} e^{-s/2H_{\epsilon_2}}, \\ & S_2 := -\int_0^{r/2} e^{-(r-u)H_{\epsilon_1}} M_{\epsilon_1} e^{-uH_0} B(X)\, e^{-s/2H_0} e^{-s/2H_{\epsilon_2}} \mathrm{d}u, \\ & S_3 := -\int_0^{s/2} e^{-r/2H_{\epsilon_1}} e^{-r/2H_0} B(X)\, e^{-vH_0} M_{\epsilon_2} e^{-(s-v)H_{\epsilon_2}} \mathrm{d}v, \\ & S_4 := \int_0^{r/2} \int_0^{s/2} e^{-(r-u)H_{\epsilon_1}} M_{\epsilon_1} e^{-uH_0} B(X)\, e^{-vH_0} M_{\epsilon_2} e^{-(s-v)H_{\epsilon_2}} \mathrm{d}v\ \mathrm{d}u. \end{aligned} \tag{262}$$

In the trace norm estimate of S_4, logarithmic terms appear similar to (256). Using Lemma 3.13, we prove

$$\Big((u,v) \mapsto \| T_1(u,v) \|_{S^1(L^2(\mathbb{R},H))} \Big) \in I_{0,0}. \tag{263}$$

For T_2 and T_3 we have to take a small detour to find a decomposition like (262). Let

$f \in \text{Dom}\left(\widehat{A_-}\right)$ and $r > 0$, then by, Lemma 2.29, we have

$$\begin{aligned}\left\{e^{-rH_\pm}A'(X)\right\}f =& e^{-r/2H_\pm}e^{-r/2H_\pm}A'(X)f = e^{-r/2H_\pm}e^{-r/2H_0}A'(X)f \\ & - e^{-r/2H_\pm}\int_0^{r/2} e^{-(r/2-u)H_\pm}M_\pm e^{-uH_0}\mathrm{d}u\ A'(X)f \\ =& e^{-r/2H_\pm}\left\{e^{-r/2H_0}A'(X)\right\}f - \int_0^{r/2} e^{-(r-u)H_\pm}M_\pm e^{-u/2H_0} \\ & \left\{e^{-u/2H_0}A'(X)\right\}f\mathrm{d}u. \qquad (264)\end{aligned}$$

A priori, the integral of the last line of (264) only converges strongly on $\text{Dom}\left(\widehat{A_-}\right)$, but the integrand can be estimated by Remark 2.20, Lemma 2.19, Proposition 2.28, Lemma 2.6 and Corollary 2.39,

$$\begin{aligned}&\left\|e^{-(r-u)H_\pm}M_\pm e^{u/2H_0}\left\{e^{-u/2H_0}A'(X)\right\}\right\|_{B(L^2(\mathbb{R},H))} \\ \leq & \left\|\left\{e^{-(r-u)H_\pm}(1+H_\pm)^\alpha\right\}\right\|_{B(L^2(\mathbb{R},H))}\left\|\left\{(1+H_\pm)^{-\alpha}(1+H_0)^\alpha\right\}\right\|_{B(L^2(\mathbb{R},H))} \\ & \left\|\left\{(1+H_0)^{-\alpha}M_\pm(1+H_0)^{-1+\alpha}\right\}\right\|_{B(L^2(\mathbb{R},H))}\left\|(1+H_0)^{1-\alpha}e^{-u/2H_0}\right\|_{B(L^2(\mathbb{R},H))} \\ & \left\|A'(X)(1+H_0)^{-1/2}\right\|_{B(L^2(\mathbb{R},H))}\left\|(1+H_0)^{1/2}e^{-u/2H_0}\right\|_{B(L^2(\mathbb{R},H))} \\ \lesssim_{t_0} & (r-u)^{-\alpha}u^{-1+\alpha}u^{-1/2} \\ \lesssim_{t_0,r} & u^{-3/2+\alpha}, \qquad (265)\end{aligned}$$

where $\alpha \in [0,1]$. If we choose $\alpha > 1/2$, (265) is integrable on $\{0 < u < r/2\}$. Since the integrand in (264) is also norm continuous in u and therefore $B\left(L^2(\mathbb{R},H)\right)$-measurable, we conclude by Lemma 2.41, that the integral in the last line of (264) converges in norm, therefore the equality in (264) extend to all $f \in L^2(\mathbb{R},H)$,

$$\begin{aligned}\left\{e^{-rH_\pm}A'(X)\right\} = e^{-r/2H_\pm}\left\{e^{-r/2H_0}A'(X)\right\} - \int_0^{r/2} e^{-(r-u)H_\pm}M_\pm e^{-u/2H_0} \\ \left\{e^{-u/2H_0}A'(X)\right\}\mathrm{d}u. \qquad (266)\end{aligned}$$

We similarly obtain

$$\partial e^{-sH_\pm} = \partial e^{-s/2H_0}e^{-s/2H_\pm} - \int_0^{s/2}\partial e^{-vH_0}M_\pm e^{-(s-v)H_\pm}\mathrm{d}v. \qquad (267)$$

Both (266) and (267) combined give us the formula

$$\begin{aligned}&T_2 = R_1 + R_2 + R_3 + R_4, \\ &R_1 := e^{-r/2H_{\epsilon_1}}\left\{e^{-r/2H_0}A'(X)\right\}\partial e^{-s/2H_0}e^{-s/2H_{\epsilon_2}},\end{aligned}$$

$$R_2 := -\int_0^{r/2} e^{-(r-u)H_{\epsilon_1}} M_{\epsilon_1} e^{-u/2H_0} \left\{e^{-u/2H_0} A'(X)\right\} \partial e^{-s/2H_0} e^{-s/2H_{\epsilon_2}} \mathrm{d}u,$$
$$R_3 := -\int_0^{s/2} e^{-r/2H_{\epsilon_1}} \left\{e^{-r/2H_0} A'(X)\right\} \partial e^{-vH_0} M_{\epsilon_2} e^{-(s-v)H_{\epsilon_2}} \mathrm{d}v,$$
$$R_4 := \int_0^{r/2}\int_0^{s/2} e^{-(r-u)H_{\epsilon_1}} M_{\epsilon_1} e^{-u/2H_0} \left\{e^{-u/2H_0} A'(X)\right\} \partial e^{-vH_0} M_{\epsilon_2} e^{-(s-v)H_{\epsilon_2}} \mathrm{d}v\ \mathrm{d}u. \tag{268}$$

With (268) we obtain estimates similar to (256) by using Lemma 3.15 and thus arrive at

$$\Big((u,v) \mapsto \|T_2(u,v)\|_{S^1(L^2(\mathbb{R},H))}\Big) \in I_{0,0}. \tag{269}$$

The operator T_3 is treated analogous to T_2 and we obtain the claimed result. ■

The next Lemma 3.18 is motivated by Lemma 2.32, in which the commutator of ∂ with the operator P_t^+ appears. This commutator is of great importance for the calculation of the trace, basically due to the fundamental theorem of calculus (c.f. Theorem 4.10).

Lemma 3.18. *Assume Hypothesis A2 (*2.11*) and either of the Hypotheses B1 (*2.12*) or B2 (*2.14*). Let $t \geq 0$. Then $\left[\partial, e^{-tH_\pm}\right] = \partial e^{-tH_\pm} - e^{-tH_\pm}\partial$ is the restriction to* $\mathrm{Dom}(\partial)$ *of a trace-class operator in $L^2(\mathbb{R},H)$, $\widetilde{U}(t)$, given by*

$$\widetilde{U}(t) := -\int_0^t e^{-sH_\pm} B(X) e^{-(t-s)H_\pm} ds \pm \int_0^t \left\{e^{-sH_\pm} A'(X)\right\} \partial e^{-(t-s)H_\pm} \mathrm{d}s$$
$$\mp \int_0^t \left\{e^{-sH_\pm}\partial\right\} A'(X) e^{-(t-s)H_\pm} \mathrm{d}s, \tag{270}$$

where $B := AA' + A'A$.
Furthermore we have for $t_0 > 0$

$$\int_0^{t_0} \left\|\left\{\left[\partial, e^{-tH_\pm}\right]\right\}\right\|_{S^1(L^2(\mathbb{R},H))} \mathrm{d}t \lesssim_{t_0} 1. \tag{271}$$

Proof. First note that for $t \geq 0$, the operator $U_0(t) := \left[\partial, e^{-tH_\pm}\right]$ is defined on $\mathrm{Dom}(\partial)$, since for $t = 0$ we have $e^{-tH_\pm} = 1$, and for $t > 0$ we know that $e^{-tH_\pm}$ maps into $\mathrm{Dom}(H_\pm) \subseteq \mathrm{Dom}(\partial)$ by Proposition 2.28.
Let $f \in \mathrm{Dom}(H_0) = \mathrm{Dom}(H_\pm)$ and $\phi(t) := U_0(t) f$. Then

$$\lim_{t\to 0}\phi(t) = \lim_{t\to 0}\partial e^{-tH_\pm} f - \lim_{t\to 0} e^{-tH_\pm}\partial f = \partial f - \partial f = 0 = \phi(0). \tag{272}$$

Here, we used that $e^{-tH_\pm}$ is strongly continuous on $\mathrm{Dom}(H_\pm)_\Gamma$, by the functional calculus of $H_\pm$. Note also that for $t > 0$, the bounded operator $U(t) := \partial e^{-tH_\pm} - \left\{e^{-tH_\pm}\partial\right\}$ exists by Lemma 2.19 and Proposition 2.28, and must be the closure of $U_0(t)$ in $L^2(\mathbb{R},H)$. Let

$t>0$, $g\in L^2(\mathbb{R},H)$ and $f\in C_c^\infty(\mathbb{R})\otimes \mathrm{Dom}\left(A_-^2\right)_\Gamma$. Then

$$\begin{aligned}&\langle g,\left\{e^{-tH_\pm}\partial\right\}H_\pm f\rangle_{L^2(\mathbb{R},H)}\\ =&-\langle \partial e^{-tH_\pm}g,M_\pm f\rangle_{L^2(\mathbb{R},H)}-\langle \partial e^{-tH_\pm}g,H_0 f\rangle_{L^2(\mathbb{R},H)}\\ =&\langle e^{-tH_\pm}g,B(X)f\rangle_{L^2(\mathbb{R},H)}+\langle e^{-tH_\pm}g,\left(A(X)^2-\widehat{A_-^2}\right)\partial f\rangle_{L^2(\mathbb{R},H)}\\ &\mp\langle \partial e^{-tH_\pm}g,A'(X)f\rangle_{L^2(\mathbb{R},H)}-\langle \partial e^{-tH_\pm}g,H_0 f\rangle_{L^2(\mathbb{R},H)}\\ =&\langle g,e^{-tH_\pm}B(X)f\rangle_{L^2(\mathbb{R},H)}+\langle\left(A(X)^2-\widehat{A_-^2}\right)e^{-tH_\pm}g,\partial f\rangle_{L^2(\mathbb{R},H)}\\ &\pm\langle g,\left\{e^{-tH_\pm}\partial\right\}A'(X)f\rangle_{L^2(\mathbb{R},H)}-\langle \partial e^{-tH_\pm}g,H_0 f\rangle_{L^2(\mathbb{R},H)}.\end{aligned}\tag{273}$$

And

$$\begin{aligned}&\langle g,H_\pm e^{-tH_\pm}\partial f\rangle_{L^2(\mathbb{R},H)}\\ =&\langle M_\pm e^{-tH_\pm}g,\partial f\rangle_{L^2(\mathbb{R},H)}+\langle H_0 e^{-tH_\pm}g,\partial f\rangle_{L^2(\mathbb{R},H)}\\ =&\langle\left(A(X)^2-\widehat{A_-^2}\right)e^{-tH_\pm}g,\partial f\rangle_{L^2(\mathbb{R},H)}\pm\langle A'(X)e^{-tH_\pm}g,\partial f\rangle_{L^2(\mathbb{R},H)}\\ &+\langle e^{-tH_\pm}g,\partial H_0 f\rangle_{L^2(\mathbb{R},H)}\\ =&\langle\left(A(X)^2-\widehat{A_-^2}\right)e^{-tH_\pm}g,\partial f\rangle_{L^2(\mathbb{R},H)}\pm\langle g,\left\{e^{-tH_\pm}A'(X)\right\}\partial f\rangle_{L^2(\mathbb{R},H)}\\ &-\langle \partial e^{-tH_\pm}g,H_0 f\rangle_{L^2(\mathbb{R},H)}.\end{aligned}\tag{274}$$

Combining equations (273) and (274), we obtain

$$\begin{aligned}&\langle g,\left(-\left\{e^{-tH_\pm}\partial\right\}H_\pm+H_\pm e^{-tH_\pm}\partial\right)f\rangle_{L^2(\mathbb{R},H)}\\ =&-\langle g,e^{-tH_\pm}B(X)f\rangle_{L^2(\mathbb{R},H)}\pm\langle g,\left(\left\{e^{-tH_\pm}A'(X)\right\}\partial-\left\{e^{-tH_\pm}\partial\right\}A'(X)\right)f\rangle_{L^2(\mathbb{R},H)}.\end{aligned}\tag{275}$$

By continuity and density of $C_c^\infty(\mathbb{R})\otimes \mathrm{Dom}\left(A_-^2\right)_\Gamma$ in $\mathrm{Dom}(H_0)_\Gamma$, we extend equation (275) to $g\in L^2(\mathbb{R},H)$ and $f\in \mathrm{Dom}(H_0)$. Therefore we have for $t>0$ and $f\in\mathrm{Dom}(H_0)$

$$\begin{aligned}&-\left\{e^{-tH_\pm}\partial\right\}H_\pm f+H_\pm e^{-tH_\pm}\partial f\\ =&-e^{-tH_\pm}B(X)f\pm\left\{e^{-tH_\pm}A'(X)\right\}\partial f\mp\left\{e^{-tH_\pm}\partial\right\}A'(X)f.\end{aligned}\tag{276}$$

Hence, we have for $t>0$ and $f\in\mathrm{Dom}(H_0)$

$$\begin{aligned}U'(t)f&=\partial_t\left(\partial e^{-tH_\pm}f-e^{-tH_\pm}\partial f\right)\\ &=-\partial e^{-tH_\pm}H_\pm f+H_\pm e^{-tH_\pm}\partial f\\ &=-U(t)H_\pm f-\left\{e^{-tH_\pm}\partial\right\}H_\pm f+H_\pm e^{-tH_\pm}\partial f\\ &=-U(t)H_\pm f-e^{-tH_\pm}B(X)f\pm\left\{e^{-tH_\pm}A'(X)\right\}\partial f\mp\left\{e^{-tH_\pm}\partial\right\}A'(X)f.\end{aligned}\tag{277}$$

For $t_0\geq t>0$ define

$$\begin{aligned}\widetilde{U}(t):=&-\int_0^t e^{-sH_\pm}B(X)e^{-(t-s)H_\pm}ds\pm\int_0^t\left\{e^{-sH_\pm}A'(X)\right\}\partial e^{-(t-s)H_\pm}\mathrm{d}s\\ &\mp\int_0^t\left\{e^{-sH_\pm}\partial\right\}A'(X)e^{-(t-s)H_\pm}\mathrm{d}s.\end{aligned}\tag{278}$$

We first note that all integrands of (278) are trace-class operators in $L^2(\mathbb{R},H)$ and trace-norm continuous (and thus $S^1\left(L^2(\mathbb{R},H)\right)$-measurable) in s for $0<s<t$, due to Lemma 3.17 and Lemma 2.37. By Lemma 2.41, the integral constituting $\widetilde{U}(t)$ converges in trace-norm for $t>0$.
We estimate each summand of (278) using Lemma 3.17, because there exists a function $g\in I_{0,0}$ of two variables, such that g is monotonously decreasing if one of the variables increases, with

$$\left\|\widetilde{U}(t)\right\|_{S^1(L^2(\mathbb{R},H))}\lesssim_{t_0}\int_0^t g(s,t-s)\,\mathrm{d}s\le\int_0^{t/2}\left(g(s,t/2)+g(t/2,s)\right)\mathrm{d}s. \tag{279}$$

Therefore, we obtain

$$\int_0^{t_0}\left\|\widetilde{U}(t)\right\|_{S^1(L^2(\mathbb{R},H))}\mathrm{d}t\lesssim_{t_0}\int_0^{t_0}\int_0^{t_0/2}\left(g(s,t/2)+g(t/2,s)\right)\mathrm{d}s\ \mathrm{d}t<\infty. \tag{280}$$

Let $f\in\mathrm{Dom}(H_\pm)$. Then

$$\begin{aligned}
&\left\|e^{-sH_\pm}B(X)\,e^{-(t-s)H_\pm}f\right\|_{L^2(\mathbb{R},H)}\\
&=\left\|e^{-sH_\pm}B(X)\,(1+H_\pm)^{-1}e^{-(t-s)H_\pm}(1+H_\pm)\,f\right\|_{L^2(\mathbb{R},H)}\lesssim\|f\|_{\mathrm{Dom}(H_\pm)_\Gamma},\\
&\left\|\left\{e^{-sH_\pm}A'(X)\right\}\partial e^{-(t-s)H_\pm}f\right\|_{L^2(\mathbb{R},H)}\\
&=\left\|\left\{e^{-sH_\pm}A'(X)\right\}\right\|_{B(L^2(\mathbb{R},H))}\left\|\partial\,(1+H_\pm)^{-1}e^{-(t-s)H_\pm}(1+H_\pm)\,f\right\|_{L^2(\mathbb{R},H)}\\
&\lesssim_{t_0}s^{-1/2}\|f\|_{\mathrm{Dom}(H_\pm)_\Gamma},\\
&\left\|\left\{e^{-sH_\pm}\partial\right\}A'(X)\,e^{-(t-s)H_\pm}f\right\|_{L^2(\mathbb{R},H)}\\
&=\left\|\left\{e^{-sH_\pm}\partial\right\}\right\|_{B(L^2(\mathbb{R},H))}\left\|A'(X)\,(1+H_\pm)^{-1}e^{-(t-s)H_\pm}(1+H_\pm)\,f\right\|_{L^2(\mathbb{R},H)}\\
&\lesssim_{t_0}s^{-1/2}\|f\|_{\mathrm{Dom}(H_\pm)_\Gamma}.
\end{aligned} \tag{281}$$

Therefore

$$\left\|\widetilde{U}(t)\,f\right\|_{L^2(\mathbb{R},H)}\lesssim_{t_0}\int_0^t s^{-1/2}\mathrm{d}s\cdot\|f\|_{\mathrm{Dom}(H_\pm)_\Gamma}\xrightarrow{t\to 0}0. \tag{282}$$

On the other hand, we have the estimates

$$\begin{aligned}
&\left\|e^{-sH_\pm}B(X)\,e^{-(t-s)H_\pm}\right\|_{B(L^2(\mathbb{R},H))}\\
&=\left\|\left\{e^{-sH_\pm}(1+H_\pm)^{1/2}\right\}\right\|_{B(L^2(\mathbb{R},H))}\left\|\left\{(1+H_\pm)^{-1/2}B(X)\,(1+H_\pm)^{-1/2}\right\}\right\|_{B(L^2(\mathbb{R},H))}\\
&\cdot\left\|(1+H_\pm)^{1/2}e^{-(t-s)H_\pm}\right\|_{B(L^2(\mathbb{R},H))}\lesssim_{t_0}s^{-1/2}(t-s)^{-1/2},\\
&\left\|\left\{e^{-sH_\pm}A'(X)\right\}\partial e^{-(t-s)H_\pm}\right\|_{B(L^2(\mathbb{R},H))}
\end{aligned}$$

$$
\begin{aligned}
&= \left\| \left\{ e^{-sH_\pm} A'(X) \right\} \right\|_{B(L^2(\mathbb{R},H))} \left\| \partial (1+H_\pm)^{-1/2} \right\|_{B(L^2(\mathbb{R},H))} \\
&\quad \cdot \left\| e^{-(t-s)H_\pm} (1+H_\pm)^{1/2} \right\|_{B(L^2(\mathbb{R},H))} \lesssim_{t_0} s^{-1/2} (t-s)^{-1/2}, \\
&\left\| \left\{ e^{-sH_\pm} \partial \right\} A'(X) e^{-(t-s)H_\pm} \right\|_{B(L^2(\mathbb{R},H))} \\
&= \left\| \left\{ e^{-sH_\pm} \partial \right\} \right\|_{B(L^2(\mathbb{R},H))} \left\| A'(X) (1+H_\pm)^{-1/2} \right\|_{B(L^2(\mathbb{R},H))} \\
&\quad \cdot \left\| e^{-(t-s)H_\pm} (1+H_\pm)^{1/2} \right\|_{B(L^2(\mathbb{R},H))} \lesssim_{t_0} s^{-1/2} (t-s)^{-1/2}.
\end{aligned}
\tag{283}
$$

This allows us to estimate

$$
\left\| \widetilde{U}(t) \right\|_{B(L^2(\mathbb{R},H))} \lesssim_{t_0} \int_0^t s^{-1/2} (t-s)^{-1/2} \, \mathrm{d}s = \pi. \tag{284}
$$

We combine (282) and (284), and, using the uniform boundedness principle, we conclude that $\widetilde{U}(t)$ converges strongly to 0 on $L^2(\mathbb{R},H)$, because $\mathrm{Dom}(H_\pm)$ is dense in $L^2(\mathbb{R},H)$. For $t>0$ and $f \in \mathrm{Dom}(H_\pm)$, we have differentiability of $\widetilde{U}(t) f$ with

$$
\widetilde{U}'(t) f = -\widetilde{U}(t) H_\pm f - e^{-tH_\pm} B(X) f \pm \left\{ e^{-tH_\pm} A'(X) \right\} \partial f \mp \left\{ e^{-tH_\pm} \partial \right\} A'(X) f. \tag{285}
$$

We note that $V(t) := U(t) - \widetilde{U}(t)$ is defined for $t \geq 0$ and is strongly continuous on $\mathrm{Dom}(H_\pm)$ with $V(0) = 0$. For $f \in \mathrm{Dom}(H_\pm)$ and $t > 0$ we have

$$
V'(t) f = -V(t) H_\pm f. \tag{286}
$$

Thus for $0 < s < t$ and $f, g \in L^2(\mathbb{R},H)$, we conclude

$$
\begin{aligned}
\partial_s \langle e^{-(t-s)H_\pm} V(s)^* f, g \rangle_{L^2(\mathbb{R},H)} &= \partial_s \langle f, V(s) e^{-(t-s)H_\pm} g \rangle_{L^2(\mathbb{R},H)} \\
&= \langle f, V(s) (H_\pm - H_\pm) e^{-(t-s)H_\pm} g \rangle_{L^2(\mathbb{R},H)} = 0.
\end{aligned}
\tag{287}
$$

Therefore, if $f \in \mathrm{Dom}(H_\pm)$ and $g \in L^2(\mathbb{R},H)$, we obtain

$$
\begin{aligned}
&\langle f, V(t) g \rangle_{L^2(\mathbb{R},H)} \\
&= \lim_{s \nearrow t} \langle f, V(s) e^{-(t-s)H_\pm} g \rangle_{L^2(\mathbb{R},H)} = \lim_{s \nearrow t} \langle e^{-(t-s)H_\pm} V(s)^* f, g \rangle_{L^2(\mathbb{R},H)} \\
&= \lim_{s \searrow 0} \langle e^{-(t-s)H_\pm} V(s)^* f, g \rangle_{L^2(\mathbb{R},H)} = \langle f, V(0) e^{-tH_\pm} g \rangle_{L^2(\mathbb{R},H)} = 0.
\end{aligned}
\tag{288}
$$

Here we used that for $0 \leq s < t$ the operator $e^{-(t-s)H_\pm}$ maps $L^2(\mathbb{R},H)$ into $\mathrm{Dom}(H_\pm)$, on which $V(s)$ is strongly continuous in $s = 0$.
Since $\mathrm{Dom}(H_\pm)$ is dense in $L^2(\mathbb{R},H)$, equation (288) implies that $V \equiv 0$ and therefore that $U(\cdot) \equiv \widetilde{U}(\cdot)$. ∎

We are now ready to derive the fundamental trace-class memberships concerning, and related to, the operators in $L^2(\mathbb{R},H)$ on the left hand side of the trace formulae (1).

Theorem 3.19. *Assume Hypothesis A1 (*2.10*) and either of the Hypotheses B1 (*2.12*) or B2 (*2.14*). Let* $t > 0$*. Then* $e^{-tH_+} - e^{-tH_-}$ *is trace-class in* $L^2(\mathbb{R}, H)$ *and for* $t_0 > 0$ *we have*

$$\int_0^{t_0} \left\| e^{-tH_+} - e^{-tH_-} \right\|_{S^1(L^2(\mathbb{R},H))} \mathrm{d}t < \infty. \tag{289}$$

*If we assume additionally Hypothesis A2 (*2.11*), we have for* $t_0 > 0$

$$\int_0^{t_0} t^{-1/2} \left\| e^{-tH_+} - e^{-tH_-} \right\|_{S^1(L^2(\mathbb{R},H))} \mathrm{d}t < \infty. \tag{290}$$

Proof. Let $0 < s < t \leq t_0$. Consider the family of operators $T(s)$ in $L^2(\mathbb{R}, H)$ given by

$$T(s) := e^{-sH_+} A'(X) e^{-(t-s)H_-}. \tag{291}$$

Lemma 3.16 implies that $T(s)$ is trace-class in $L^2(\mathbb{R}, H)$. By Lemma 2.37 we infer that $s \mapsto T(s)$ is $S^1\left(L^2(\mathbb{R}, H)\right)$-norm continuous for $s \in (0, t)$ and therefore $S^1\left(L^2(\mathbb{R}, H)\right)$-measurable.
Also by Lemma 3.16 (and monotony,) we obtain

$$\begin{aligned}
&\int_0^t \|T(s)\|_{S^1(L^2(\mathbb{R},H))} \mathrm{d}s \\
\leq &\int_0^{t/2} \left(\left\| e^{-sH_+} A'(X) e^{-t/2H_-} \right\|_{S^1(L^2(\mathbb{R},H))} + \left\| e^{-t/2H_+} A'(X) e^{-sH_-} \right\|_{S^1(L^2(\mathbb{R},H))} \right) \mathrm{d}s \\
<&\infty.
\end{aligned} \tag{292}$$

Therefore, by Lemma 2.41 the integral

$$\int_0^t e^{-sH_+} A'(X) e^{-(t-s)H_-} \mathrm{d}s$$

converges in $S^1\left(L^2(\mathbb{R}, H)\right)$.
On the other hand, we have for $f \in L^2(\mathbb{R}, H)$ that

$$-2 \int_0^t e^{-sH_+} A'(X) e^{-(t-s)H_-} \mathrm{d}s\ f = - \int_0^t e^{-sH_+} (H_+ - H_-) e^{-(t-s)H_-} f \mathrm{d}s \tag{293}$$

$$= \int_0^t \partial_s \left(e^{-sH_+} e^{-(t-s)H_-} f \right) \mathrm{d}s \tag{294}$$

$$= \left[e^{-sH_+} e^{-(t-s)H_-} f \right]_{s=0}^{s=t} = \left(e^{-tH_+} - e^{-tH_-} \right) f. \tag{295}$$

Thus, by estimate (292), Lemma 2.41, and equation (293), the operator $e^{-tH_+} - e^{-tH_-}$ is trace-class in $L^2(\mathbb{R}, H)$, for $t > 0$. We furthermore obtain

$$\begin{aligned}
&\int_0^{t_0} \left\| e^{-tH_+} - e^{-tH_-} \right\|_{S^1(L^2(\mathbb{R},H))} \mathrm{d}t \\
\leq &2 \int_0^{t_0} \int_0^{t_0/2} \left(\left\| e^{-sH_+} A'(X) e^{-t/2H_-} \right\|_{S^1(L^2(\mathbb{R},H))} \right. \\
&\qquad \left. + \left\| e^{-t/2H_+} A'(X) e^{-sH_-} \right\|_{S^1(L^2(\mathbb{R},H))} \right) \mathrm{d}s\ \mathrm{d}t < \infty,
\end{aligned} \tag{296}$$

by Lemma 3.16.
If we assume additionally Hypothesis A2 (2.11), we obtain

$$\begin{aligned}
&\int_0^{t_0} t^{-1/2} \left\|e^{-tH_+} - e^{-tH_-}\right\|_{S^1(L^2(\mathbb{R},H))} \mathrm{d}t \\
\leq& 2\int_0^{t_0}\int_0^{t_0/2} t^{-1/2} \left(\left\|e^{-sH_+} A'(X) e^{-t/2H_-}\right\|_{S^1(L^2(\mathbb{R},H))}\right. \\
&\qquad\qquad \left. + \left\|e^{-t/2H_+} A'(X) e^{-sH_-}\right\|_{S^1(L^2(\mathbb{R},H))}\right) \mathrm{d}s\ \mathrm{d}t < \infty, \qquad (297)
\end{aligned}$$

by Lemma 3.16. ■

Theorem 3.20. *Assume Hypothesis A1 (2.10) and either of the Hypotheses B1 (2.12) or B2 (2.14). Let $t > 0$. Then $H_+e^{-tH_+} - H_-e^{-tH_-}$ is trace-class in $L^2(\mathbb{R}, H)$ and for $t_0 > 0$ we have*

$$\int_0^{t_0} t \left\|H_+e^{-tH_+} - H_-e^{-tH_-}\right\|_{S^1(L^2(\mathbb{R},H))} \mathrm{d}t < \infty. \qquad (298)$$

If we assume additionally Hypothesis A2 (2.11), we have for $t_0 > 0$

$$\int_0^{t_0} t^{1/2} \left\|H_+e^{-tH_+} - H_-e^{-tH_-}\right\|_{S^1(L^2(\mathbb{R},H))} \mathrm{d}t < \infty. \qquad (299)$$

Proof. We obtain for $t > 0$

$$\begin{aligned}
H_+e^{-tH_+} - H_-e^{-tH_-} =& \left(e^{-t/2H_+} - e^{-t/2H_-}\right) H_+e^{-t/2H_+} + e^{-t/2H_-}(H_+ - H_-) e^{-t/2H_+} \\
&+ e^{-t/2H_-} H_- \left(e^{-t/2H_+} - e^{-t/2H_-}\right) \\
=& \left(e^{-t/2H_+} - e^{-t/2H_-}\right) H_+e^{-t/2H_+} + 2e^{-t/2H_-} A'(X) e^{-t/2H_+} \\
&+ H_-e^{-t/2H_-} \left(e^{-t/2H_+} - e^{-t/2H_-}\right). \qquad (300)
\end{aligned}$$

Equation (300) together with Theorem 3.19 and Lemma 3.16 imply that $H_+e^{-tH_+} - H_-e^{-tH_-}$ is trace-class in $L^2(\mathbb{R}, H)$.
Let

$$g(r, s) := 2\left\|e^{r/2H_-} A'(X) e^{-s/2H_+}\right\|_{S^1(L^2(\mathbb{R},H))}. \qquad (301)$$

For $t_0 > 0$ we estimate by equation (300)

$$\begin{aligned}
&\int_0^{t_0} t \left\|H_+e^{-tH_+} - H_-e^{-tH_-}\right\|_{S^1(L^2(\mathbb{R},H))} \mathrm{d}t \\
\lesssim_{t_0}& \int_0^{t_0} t \left\|e^{-t/2H_+} - e^{-t/2H_-}\right\|_{S^1(L^2(\mathbb{R},H))} \cdot t^{-1}\mathrm{d}t + \int_0^{t_0} tg(t, t)\,\mathrm{d}t
\end{aligned}$$

$$+\int_0^{t_0} t\cdot t^{-1}\cdot\left\|e^{-t/2H_+}-e^{-t/2H_-}\right\|_{S^1(L^2(\mathbb{R},H))}\mathrm{d}t$$
$$\leq 2\int_0^{t_0}\left\|e^{-t/2H_+}-e^{-t/2H_-}\right\|_{S^1(L^2(\mathbb{R},H))}\mathrm{d}t+\int_0^{t_0} t\cdot t^{-1}\int_0^t g(t,s)\,\mathrm{d}s\;\mathrm{d}t$$
$$\leq 2\int_0^{t_0}\left\|e^{-t/2H_+}-e^{-t/2H_-}\right\|_{S^1(L^2(\mathbb{R},H))}\mathrm{d}t+\int_0^{t_0}\int_0^{t_0} g(t,s)\,\mathrm{d}s\;\mathrm{d}t<\infty. \tag{302}$$

Here we used the trace-norm estimates from Theorem 3.19, Lemma 3.16, the norm estimate from Corollary 2.39 and the monotony of g.
Analogously one obtains, if additionally Hypothesis (2.11) is assumed, that

$$\int_0^{t_0} t^{1/2}\left\|H_+e^{-tH_+}-H_-e^{-tH_-}\right\|_{S^1(L^2(\mathbb{R},H))}\mathrm{d}t<\infty. \tag{303}$$

■

In view of Lemma 2.32, we also obtain the following Theorem 3.21 for the commutator of ∂ and P_t^+.

Theorem 3.21. *Assume Hypothesis A2* (2.11) *and either of the Hypotheses B1* (2.12) *or B2* (2.14)*. Let $t>0$. Then the operators $\{[\partial,P_t^+]\}$ and $\{[A(X),P_t^+]\}$ are trace-class in $L^2(\mathbb{R},H)$, and for $t_0>0$,*

$$\int_0^{t_0} t^{1/2}\left\|\{[A'(X),P_t^+]\}\right\|_{S^1(L^2(\mathbb{R},H))}\mathrm{d}t<\infty,$$
$$\int_0^{t_0} t^{1/2}\left\|\{[\partial,P_t^+]\}\right\|_{S^1(L^2(\mathbb{R},H))}\mathrm{d}t<\infty. \tag{304}$$

Proof. Let $f\in C_c^\infty(\mathbb{R})\otimes\mathrm{Dom}(A_-)$. Then for $t>0$ we obtain by Lemma 2.40

$$\begin{aligned}\partial e^{-t/2H_-}D^*f&=\left\{\left[\partial,e^{-t/2H_-}\right]\right\}D^*f+\left\{e^{-t/2H_-}\partial\right\}D^*f\\&=\left\{\left[\partial,e^{-t/2H_-}\right]\right\}D^*f+e^{-t/2H_-}\partial D^*f\\&=\left\{\left[\partial,e^{-t/2H_-}\right]\right\}D^*f+e^{-t/2H_-}D^*\partial f+e^{-t/2H_-}A'(X)f\\&=\left\{\left[\partial,e^{-t/2H_-}\right]\right\}D^*f+D^*e^{-t/2H_+}\partial f+e^{-t/2H_-}A'(X)f.\end{aligned} \tag{305}$$

Note that the left hand side and the last right hand side are bounded operators, from $\mathrm{Dom}(D_0)_\Gamma$ to $L^2(\mathbb{R},H)$, applied to f. Since $C_c^\infty(\mathbb{R})\otimes\mathrm{Dom}(A_-)$ is dense in $\mathrm{Dom}(D_0)_\Gamma$, we conclude by continuity that for $f\in\mathrm{Dom}(D_0)$, we have

$$\partial e^{-t/2H_-}D^*f=\left\{\left[\partial,e^{-t/2H_-}\right]\right\}D^*f+D^*e^{-t/2H_+}\partial f+e^{-t/2H_-}A'(X)f. \tag{306}$$

Since the operator $e^{-t/2H_+}$ maps H into $\mathrm{Dom}(D_0)$, we obtain for $f\in\mathrm{Dom}(\partial)$

$$\partial e^{-t/2H_-}D^*e^{-t/2H_+}f=\left\{\left[\partial,e^{-t/2H_-}\right]\right\}D^*e^{-t/2H^+}f+e^{-t/2H_-}A'(X)e^{-t/2H_+}f$$

$$+ D^* e^{-t/2H_+} \left\{ \left[\partial, e^{-t/2H_+} \right] \right\} f + D^* e^{-tH_+} \partial f \tag{307}$$

Lemma 2.40 implies that

$$P_t^+ = e^{-t/2H_-} D^* e^{-t/2H_+}. \tag{308}$$

Therefore equation (307) yields

$$\left\{ \left[\partial, P_t^+ \right] \right\} = \left\{ \left[\partial, e^{-t/2H_-} \right] \right\} P_{t/2}^+ + e^{-t/2H_-} A' (X) e^{-t/2H_+} + P_{t/2}^+ \left\{ \left[\partial, e^{-t/2H_+} \right] \right\}, \tag{309}$$

where all three summands are trace-class operators in $L^2 (\mathbb{R}, H)$, by Lemma 3.16 and Lemma 3.18.
Theorem 3.20 together with Lemma 2.32 then imply that also $\left\{ \left[A (X), P_t^+ \right] \right\}$ must be trace-class in $L^2 (\mathbb{R}, H)$.
Let

$$g (r, s) := \left\| e^{-r/2H_-} A' (X) e^{-s/2H_+} \right\|_{S^1(L^2(\mathbb{R},H))}. \tag{310}$$

The function g is monotonously decreasing in both arguments and, by Lemma 3.16, a function in $I_{-1/2,0}$. Thus for $t_0 > 0$ we have

$$\begin{aligned} \int_0^{t_0} t^{1/2} g (t, t) \,\mathrm{d}t &\leq \int_0^{t_0} t^{1/2} \cdot t^{-1} \int_0^t g (t, s) \,\mathrm{d}s \;\mathrm{d}t \\ &\leq \int_0^{t_0} \int_0^{t_0} t^{-1/2} g (t, s) \,\mathrm{d}s \;\mathrm{d}t < \infty. \end{aligned} \tag{311}$$

Since $\mathrm{Dom}\,(D)_\Gamma = \mathrm{Dom}\,(H_\pm)_\Gamma$ holds, by Proposition 2.28, Corollary 2.39 implies for $t_0 \geq t > 0$,

$$\left\| P_{t/2}^+ \right\|_{B(L^2(\mathbb{R},H))} \lesssim_{t_0} t^{-1/2}. \tag{312}$$

Equation (309) together with the estimates (311) and (312) and Lemma 3.18, enable us to make the following estimate for $t_0 > 0$:

$$\begin{aligned} &\int_0^{t_0} t^{1/2} \left\| \left\{ \left[\partial, P_t^+ \right] \right\} \right\|_{S^1(L^2(\mathbb{R},H))} \mathrm{d}t \\ \lesssim_{t_0} &\int_0^{t_0} t^{1/2} g (t, t) \,\mathrm{d}t + 2 \int_0^{t_0} \left\| \left\{ \left[\partial, e^{-t/2H_+} \right] \right\} \right\|_{S^1(L^2(\mathbb{R},H))} \mathrm{d}t < \infty. \end{aligned} \tag{313}$$

Since Theorem 3.20 implies for $t_0 > 0$

$$\int_0^{t_0} t^{1/2} \left\| H_+ e^{-tH_+} - H_- e^{-tH_-} \right\|_{S^1(L^2(\mathbb{R},H))} \mathrm{d}t < \infty, \tag{314}$$

we conclude, by Lemma 2.32, that also

$$\int_0^{t_0} t^{1/2} \left\| \left\{ \left[A' (X), P_t^+ \right] \right\} \right\|_{S^1(L^2(\mathbb{R},H))} \mathrm{d}t < \infty. \tag{315}$$

■

We close this subsection by giving the analogous result for the operator Q_t^+ instead of P_t^+.

Theorem 3.22. *Assume Hypothesis A2 (*2.11*) and either of the Hypotheses B1 (*2.12*) or B2 (*2.14*). Let $t, \epsilon > 0$, then*

$$e^{-\epsilon H_0}\left(e^{-tH_+} - e^{-tH_-}\right)e^{-\epsilon H_0} = -te^{-\epsilon H_0}\left[\partial, Q_t^+\right]e^{-\epsilon H_0} - te^{-\epsilon H_0}\left[A\left(X\right), Q_t^+\right]e^{-\epsilon H_0}. \tag{316}$$

The operators

$$e^{-\epsilon H_0}\left[\partial, Q_t^+\right]e^{-\epsilon H_0}$$

and

$$e^{-\epsilon H_0}\left[A\left(X\right), Q_t^+\right]e^{-\epsilon H_0}$$

are trace-class in $L^2\left(\mathbb{R}, H\right)$.

Proof. We recall the definition of the function γ in Definition 2.33 and note that for $z \in \mathbb{C}$ and $t > 0$, we have

$$e^{-tz} - 1 = -tz\gamma\left(tz\right). \tag{317}$$

Therefore we conclude, by Lemma 2.40, for $f \in \mathrm{Dom}\left(D_0\right)$

$$\begin{aligned}\left(e^{-tH_+} - e^{-tH_-}\right)f &= \left(e^{-tH_+} - 1 + 1 - e^{-tH_-}\right)f = -t\left(H_+\gamma\left(tH_+\right) - H_-\gamma\left(tH_-\right)\right)f \\ &= -t\left[D, D^*\gamma\left(tH_+\right)\right]f = -t\left[\partial, Q_t^+\right]f - t\left[A\left(X\right), Q_t^+\right]f.\end{aligned} \tag{318}$$

For $\epsilon > 0$ we find, using the formula from Remark 2.34,

$$\begin{aligned}&e^{-\epsilon H_0}\left(e^{-tH_+} - e^{-tH_-}\right)e^{-\epsilon H_0} \\ =& - te^{-\epsilon H_0}\left[\partial, Q_t^+\right]e^{-\epsilon H_0} - te^{-\epsilon H_0}\left[A\left(X\right), Q_t^+\right]e^{-\epsilon H_0} \\ =& - te^{-\epsilon H_0}\left[\partial, D^*\right]\gamma\left(tH_+\right)e^{-\epsilon H_0} - te^{-\epsilon H_0}D^*\left[\partial, \gamma\left(tH_+\right)\right]e^{-\epsilon H_0} \\ &- te^{-\epsilon H_0}\left[A\left(X\right), Q_t^+\right]e^{-\epsilon H_0} \\ =& - te^{-\epsilon H_0}A'\left(X\right)\left(1 + H_0\right)^{-1}\left(1 + H_0\right)\left(1 + H_+\right)^{-1}\left(\gamma\left(tH_+\right) + 1/t\left(1 - e^{-tH_+}\right)\right)e^{-\epsilon H_0} \\ &- t\left\{e^{-\epsilon H_0}D^*\right\}\left\{\left[\partial, \gamma\left(tH_+\right)\right]\right\}e^{-\epsilon H_0} \\ &- te^{-\epsilon H_0}\left[A\left(X\right), Q_t^+\right]e^{-\epsilon H_0}.\end{aligned} \tag{319}$$

Since

$$e^{-\epsilon H_0}A'\left(X\right)\left(1 + H_0\right)^{-1} = \left(1 + H_0\right)e^{-\epsilon H_0}\left(1 + H_0\right)^{-1}A'\left(X\right)\left(1 + H_0\right)^{-1}, \tag{320}$$

the first summand of the last line of (319),

$$-te^{-\epsilon H_0}A'\left(X\right)\left(1 + H_0\right)^{-1}\left(1 + H_0\right)\left(1 + H_+\right)^{-1}\left(\gamma\left(tH_+\right) + 1/t\left(1 - e^{-tH_+}\right)\right)e^{-\epsilon H_0},$$

is a product of a trace-class operator in $L^2(\mathbb{R}, H)$, by Lemma 3.14, and of bounded operators in $L^2(\mathbb{R}, H)$, by Proposition 2.28, and therefore trace-class in $L^2(\mathbb{R}, H)$.
By the functional calculus we further note that

$$t^{-1}\int_0^t e^{-sH_+}\mathrm{d}s = \gamma(tH_+), \tag{321}$$

where the integral converges in the strong operator topology. We conclude that for $f \in \mathrm{Dom}(D_0)$,

$$[\partial, \gamma(tH_+)] f = t^{-1}\int_0^t \left[\partial, e^{-sH_+}\right] f\mathrm{d}s = t^{-1}\int_0^t \left\{\left[\partial, e^{-sH_+}\right]\right\}\mathrm{d}sf, \tag{322}$$

where the last integral converges strongly. On the other hand, by Lemma 3.18, the operator $\left\{\left[\partial, e^{-sH_+}\right]\right\}$ is trace-class for $s > 0$ and, in regard of

$$\left\{\left[\partial, e^{-(s+h)H_+}\right]\right\} - \left\{\left[\partial, e^{-sH_+}\right]\right\} = \left\{\left[\partial, e^{-s/2H_+}\right]\right\}\left(e^{-(h+s/2)H_+} - e^{-s/2H_+}\right), \tag{323}$$

and Lemma 2.37, $S^1\left(L^2(\mathbb{R}, H)\right)$-continuous on $s > 0$ (and thus is $S^1\left(L^2(\mathbb{R}, H)\right)$ -measurable). By Lemma 3.18 ,the trace norm of $\left\{\left[\partial, e^{-sH_+}\right]\right\}$ is integrable on any compact interval $[0, t_0] \ni s$, for $t_0 > 0$, and thus, by Lemma 2.41, we may conclude that the last integral of (322) must converge in $S^1\left(L^2(\mathbb{R}, H)\right)$.
Therefore $\{[\partial, \gamma(tH_+)]\} \in S^1\left(L^2(\mathbb{R}, H)\right)$.
By Theorem 3.19 the operator $e^{-tH_+} - e^{-tH_-}$ is also trace-class in $L^2(\mathbb{R}, H)$. In summary, the first line of (319) is trace-class as well as the first and second summand of the last line of (319). Thus also the remaining third summand,

$$-te^{-\epsilon H_0}\left[A(X), Q_t^+\right]e^{-\epsilon H_0},$$

must be trace-class in $L^2(\mathbb{R}, H)$.
In regard of the second line of (319) we conclude that also

$$-te^{-\epsilon H_0}\left[\partial, Q_t^+\right]e^{-\epsilon H_0}$$

is trace-class in $L^2(\mathbb{R}, H)$. ■

3.4 The spectral shift function of the pair (H_+, H_-)

In Theorem 3.19 we have shown that the difference $e^{-tH_+} - e^{-tH_-}$ is trace-class in $L^2(\mathbb{R}, H)$ for $t > 0$. In essence, because $e^{-t\cdot}$ is bijective on the spectra of $H_\pm$, we may construct the spectral shift function of the pair (H_+, H_-), by the following procedure taken from [38].

Let $t > 0$ and let $\psi_t(\lambda) := e^{-t\lambda}$. Then $\psi_t'(\lambda) = -te^{-t\lambda} < 0$, for all $\lambda \in \mathbb{R}$. ψ_t is bounded on the non-negative numbers and is twice continuously differentiable and one-to-one on $\mathbb{R}$. Since $\sigma(H_+) \cup \sigma(H_-) \subseteq [0, \infty)$, and $\psi_t(H_+) - \psi_t(H_-)$ is trace-class in $L^2(\mathbb{R}, H)$ for $t > 0$, according to Theorem 3.19, we see that [38, Condition 8.11.2] is fulfilled with $\Omega = [0, \infty)$ covering itself and ψ_t as ϕ. According to equation [38, (8.11.2)], we may therefore define a spectral shift function of the pair (H_+, H_-) in the following way.

Definition 3.23. Let $t > 0$. Then define the spectral shift function $\xi(\cdot, H_+, H_-)$ of the pair (H_+, H_-) by

$$\begin{aligned} \xi(\lambda, H_+, H_-) &:= -\xi\left(e^{-t\lambda}, e^{-tH_+}, e^{-tH_-}\right), \quad \text{for } \lambda \geq 0, \\ \xi(\lambda, H_+, H_-) &:= 0 \quad \text{for } \lambda < 0, \end{aligned} \tag{324}$$

where $\xi\left(\cdot, e^{-tH_+}, e^{-tH_-}\right)$ is the spectral shift function of the pair $\left(e^{-tH_+}, e^{-tH_-}\right)$ defined by [38, Theorem 8.2.1], i.e.

$$\begin{aligned} &\xi\left(\lambda, e^{-tH_+}, e^{-tH_-}\right) \\ :=&\pi^{-1} \lim_{\epsilon \searrow 0} \Im\left(\log\left(\det{}_{L^2(\mathbb{R},H)}\left(1 + \left(e^{-tH_+} - e^{-tH_-}\right)\left(e^{-tH_-} - \lambda - i\epsilon\right)^{-1}\right)\right)\right), \end{aligned} \tag{325}$$

where the branches of $\log\det{}_{L^2(\mathbb{R},H)}$ in the upper and lower half-plane are chosen such that

$$\lim_{|\Im(z)| \to \infty} \log\left(\det{}_{L^2(\mathbb{R},H)}\left(1 + \left(e^{-tH_+} - e^{-tH_-}\right)\left(e^{-tH_-} - z\right)^{-1}\right)\right) = 0. \tag{326}$$

Remark 3.24. In accordance with inequality [38, (8.2.6)] we have, by the transformation rule, that

$$\int_0^\infty |\xi(\lambda, H_+, H_-)|\, e^{-t\lambda} \mathrm{d}\lambda \leq t^{-1} \left\| e^{-tH_+} - e^{-tH_-} \right\|_{S^1(L^2(\mathbb{R},H))} < \infty. \tag{327}$$

Additionally the trace formula,

$$\operatorname{tr}_{L^2(\mathbb{R},H)}\left(f(H_+) - f(H_-)\right) = \int_0^\infty f'(\lambda)\, \xi(\lambda, H_1, H_0)\, \mathrm{d}\lambda, \tag{328}$$

holds for $f \in C_c^\infty(\mathbb{R})$ by [38, Lemma 8.11.3].

We may improve on the properties of $\xi(\cdot, H_+, H_-)$ in Remark 3.24 and the amenable functions f for the trace formula, by introducing another spectral shift function, $\tilde{\xi}(\cdot, H_+, H_-)$.

Lemma 3.25. *Let*

$$(s,t) \mapsto g(s,t) := \int_{\mathbb{R}} \left\| e^{-tA_0^2} A'(x)\, e^{-sA_0^2} \right\|_{S^1(H)} \mathrm{d}x \in I_{1/4,1/4}. \tag{329}$$

Then

$$(1 + H_+)^{-1} - (1 + H_-)^{-1} \in S^1\left(L^2(\mathbb{R}, H)\right). \tag{330}$$

Proof. Recall that $\operatorname{Dom}(H_\pm) = \operatorname{Dom}(H_0)$ and $H_+ - H_- = 2\, A'(X)|_{\operatorname{Dom}(H_0)}$. Then, by the resolvent identity, we have

$$\begin{aligned} (H_+ + 1)^{-1} - (H_- + 1)^{-1} &= -2\,(H_+ + 1)^{-1} A'(X)\,(H_- + 1)^{-1} \\ &= -2 \int_0^\infty \int_0^\infty e^{-s} e^{-t} e^{-tH_+} A'(X)\, e^{-sH_-} \mathrm{d}s\ \mathrm{d}t, \end{aligned} \tag{331}$$

where we note that the integral converges in $S^1\left(L^2\left(\mathbb{R},H\right)\right)$. Indeed, the integrand is a continuous family of trace-class operators in $L^2\left(\mathbb{R},H\right)$, by Lemma 3.16, in both $s,t>0$, and therefore is $S^1\left(L^2\left(\mathbb{R},H\right)\right)$-measurable. Lemma 3.16 also implies

$$(s,t)\mapsto \left\|e^{-tH_+}A'\left(X\right)e^{-sH_-}\right\|_{S^1(L^2(\mathbb{R},H))}\in I_{0,0}. \tag{332}$$

Since

$$(s,t)\mapsto \left\|e^{-tH_+}A'\left(X\right)e^{-sH_-}\right\|_{S^1(L^2(\mathbb{R},H))}, \tag{333}$$

is monotonously decreasing if t and s increase, minding the factor $e^{-s}e^{-t}$, we conclude that

$$(s,t)\mapsto \left\|e^{-s}e^{-t}e^{-tH_+}A'\left(X\right)e^{-sH_-}\right\|_{S^1(L^2(\mathbb{R},H))}\in L^1\left(\left[0,\infty\right)^2\right). \tag{334}$$

Therefore, $\left(H_++1\right)^{-1}-\left(H_-+1\right)^{-1}$ is trace-class in $L^2\left(\mathbb{R},H\right)$. ■

We introduce the following "alternative" construction of a spectral shift function of the pair $\left(H_+,H_-\right)$, however we will show later that both spectral shift functions subordinated to $\left(H_+,H_-\right)$ coincide a.e..

Definition 3.26. Define the spectral shift function $\tilde{\xi}\left(\cdot,H_+,H_-\right)$ of the pair $\left(H_+,H_-\right)$ by

$$\begin{aligned}&\tilde{\xi}\left(\lambda,H_+,H_-\right):=-\xi\left(\left(\lambda+1\right)^{-1},\left(H_++a\right)^{-1},\left(H_-+1\right)^{-1}\right),\quad\text{for }\lambda\geq 0,\\&\tilde{\xi}\left(\lambda,H_+,H_-\right):=0,\quad\text{for }\lambda<0,\end{aligned} \tag{335}$$

where $\xi\left(\cdot,\left(H_++1\right)^{-1},\left(H_-+1\right)^{-1}\right)$ is the spectral shift function of the pair $\left(\left(H_++1\right)^{-1},\left(H_-+1\right)^{-1}\right)$, defined by [38, Theorem 8.2.1], i.e.

$$\begin{aligned}&\xi\left(\lambda,\left(H_++1\right)^{-1},\left(H_-+1\right)^{-1}\right)\\:=&\pi^{-1}\lim_{\epsilon\searrow 0}\Im\left(\log\left(\det{}_{L^2(\mathbb{R},H)}\left(1+\left(\left(H_++1\right)^{-1}-\left(H_-+1\right)^{-1}\right)\right.\right.\right.\\&\left.\left.\left.\left(\left(H_-+1\right)^{-1}-\lambda-i\epsilon\right)^{-1}\right)\right)\right),\end{aligned} \tag{336}$$

where the branches of $\log\det{}_{L^2(\mathbb{R},H)}$ in the upper and lower half-plane are chosen such that

$$\lim_{|\Im(z)|\to\infty}\log\left(\det{}_{L^2(\mathbb{R},H)}\left(1+\left(\left(H_++1\right)^{-1}-\left(H_-+1\right)^{-1}\right)\left(\left(H_-+1\right)^{-1}-z\right)^{-1}\right)\right)=0. \tag{337}$$

Lemma 3.27. *Let f be a twice differentiable function on $\mathbb{R}$ with locally bounded second derivative and satisfying for some $\delta>0$ the condition*

$$\left(\left(\lambda+1\right)^2f'\left(\lambda\right)\right)'\lesssim_\delta\left|\lambda\right|^{-1-\delta},\quad\textit{for }\lambda\geq 0. \tag{338}$$

Then the trace formula

$$\operatorname{tr}_{L^2(\mathbb{R},H)}\left(f\left(H_+\right)-f\left(H_-\right)\right)=\int_0^{\infty} f'\left(\lambda\right)\tilde{\xi}\left(\lambda,H_+,H_-\right)\mathrm{d}\lambda \tag{339}$$

holds and we have $\tilde{\xi}\left(\cdot,H_+,H_-\right)\in L^1\left(\mathbb{R},\left(\lambda^2+1\right)^{-1}\mathrm{d}\lambda\right)$.

Proof. As we have seen before, we prove the statement by showing that [38, Theorem 8.11.5] can be applied. Let $\phi\left(\lambda\right):=\left(\lambda+1\right)^{-1}$. Then $\phi'\left(\lambda\right)=-\left(\lambda+1\right)^{-2}<0$ for all $\lambda\geq 0$. ϕ is bounded on the non-negative numbers and is twice continuously differentiable in a neighbourhood of $[0,\infty)$. Since $\sigma\left(H_+\right)\cup\sigma\left(H_-\right)\subseteq[0,\infty)$, we see that [38, Condition 8.11.2] is satisfied with $\Omega=[0,\infty)$ covering itself. This fixes, by equation [38, (8.11.4)], the spectral shift function $\tilde{\xi}\left(\cdot,H_+,H_-\right)$ of $\left(H_+,H_-\right)$ on $\Omega=[0,\infty)$. The choice of $\tilde{\xi}\left(\lambda,H_+,H_-\right)=0$ for $\lambda<0$ is then in accordance with the fact, that the operators $H_\pm$ are bounded below by 0, and in accordance with the last paragraph in [38, §11] before [38, Theorem 8.11.5]. We see that the conditions on f are also directly derived from [38, Theorem 8.11.5] with $\phi\left(\lambda\right)=\left(\lambda+1\right)^{-1}$. Therefore the trace formula holds as stated.
For the L^1-membership of $\tilde{\xi}\left(\cdot,H_+,H_-\right)$, we see that this again follows by transformation rule and inequality [38, (8.2.6)],

$$\begin{aligned}&\int_{\mathbb{R}}\left|\tilde{\xi}\left(\lambda,H_+,H_-\right)\right|\left(\lambda^2+1\right)^{-1}\mathrm{d}\lambda\\ \lesssim&\int_0^{\infty}\left|\tilde{\xi}\left(\lambda,H_+,H_-\right)\right|\left|\phi'\left(\lambda\right)\right|\mathrm{d}\lambda\leq C\left\|\left(H_++1\right)^{-1}-\left(H_-+1\right)^{-1}\right\|_{S^1(L^2(\mathbb{R},H))}<\infty.\end{aligned} \tag{340}$$

■

Lemma 3.28. $\xi\left(\cdot,H_+,H_-\right)=\tilde{\xi}\left(\cdot,H_+,H_-\right)$ *a.e..*

Proof. Let $f\in C_c^{\infty}\left(\mathbb{R}\right)$. The conditions in Lemma 3.27 are satisfied, and we therefore have the trace formula with both spectral shift functions $\xi\left(\cdot,H_+,H_-\right)$ and $\tilde{\xi}\left(\cdot,H_+,H_-\right)$ by Remark 3.24 and Lemma 3.27, i.e.

$$\int_0^{\infty} f'\left(\lambda\right)\xi\left(\lambda,H_+,H_-\right)\mathrm{d}\lambda=\operatorname{tr}_{L^2(\mathbb{R},H)}\left(f\left(H_+\right)-f\left(H_-\right)\right)=\int_0^{\infty} f'\left(\lambda\right)\tilde{\xi}\left(\lambda,H_+,H_-\right)\mathrm{d}\lambda. \tag{341}$$

Therefore we have

$$\begin{aligned}&\int_{\mathbb{R}} f'\left(\lambda\right)\left(\xi\left(\lambda,H_+,H_-\right)-\tilde{\xi}\left(\lambda,H_+,H_-\right)\right)\mathrm{d}\lambda\\ =&\int_0^{\infty} f'\left(\lambda\right)\left(\xi\left(\lambda,H_+,H_-\right)-\tilde{\xi}\left(\lambda,H_+,H_-\right)\right)\mathrm{d}\lambda=0,\end{aligned} \tag{342}$$

for arbitrary $f\in C_c^{\infty}\left(\mathbb{R}\right)$, which implies by the Du Bois-Raymond Lemma (c.f. [27, Theorem 6.11]), that $\xi\left(\cdot,H_+,H_-\right)-\tilde{\xi}\left(\cdot,H_+,H_-\right)$ equals a constant a.e. on $\mathbb{R}$. Since $\xi\left(\lambda,H_+,H_-\right)=0=\tilde{\xi}\left(\lambda,H_+,H_-\right)$, for $\lambda<0$ we conclude that the functions must be identical a.e.. ■

Remark 3.29. Lemma 3.28 implies immediately that all statements made in Lemma 3.27 for $\tilde{\xi}(\cdot, H_+, H_-)$ hold ad verbatim for $\xi(\cdot, H_+, H_-)$.

4 Trace identities

In this chapter, which forms together with the previous chapter 3 the bulk of this work, we derive the trace formulae (1).

The general strategy is to use appropriate $B(H)$-valued integral kernels of the operators P_t^+ and Q_t^+, which stand in relation to the left hand side of the trace formulae (1), in accordance with the decompositions in Lemma 2.32, and Theorem 3.22 respectively. We then calculate the traces as integrals over the diagonal of the H-traces of the total derivative of these kernels, allowing us to calculate the trace in $L^2(\mathbb{R}, H)$ as the H-trace of the difference of the limits of these kernels approaching $\pm\infty$, respectively, on the diagonal. The remaining commutators involving $A(X)$ from the decompositions in Lemma 2.32 and Theorem 3.22 then are shown to give no contribution to the $L^2(\mathbb{R}, H)$-trace, which finishes the proof of the trace formulae (1).

Let us begin this chapter by highlighting the importance of the Brüning Seeley Trace Lemma, which was shown in the annex of [10]. This result enables us to generalize the elementary idea of calculating the trace by adding the entries of the diagonal of a matrix to (operator valued-) integral kernels integrated over the diagonal. Note that a similar result dealing with scalar valued integral kernels is usually referred to as Mercer's theorem (c.f. Mercer's Theorem in [40, Satz VI.4.2]).

4.1 The Brüning Seeley Trace Lemma

At this point we have all trace-class operators at hand, which we need to calculate the trace of $H_+e^{-tH_+} - H_-e^{-tH_-}$ for $t > 0$. What is still needed, is an operator-valued version of Mercer's theorem, as we want to calculate the trace by integrating the trace in H of its operator-valued kernel over the diagonal. The result we are looking for is known as Brüning and Seeley's Trace Lemma ([10]), which we will cite below with some minor changes fitting our notation.

Theorem 4.1 (Brüning/Seeley Trace Lemma)**.** *Let T be a trace-class operator in $L^2(\mathbb{R}, H)$. Then T has a kernel $t(x,y)$ such that*

$$Tf(x) = \int_{\mathbb{R}} t(x,y) f(y) \,\mathrm{d}y, \tag{343}$$

and

$$h \mapsto t(\cdot, \cdot + h) \tag{344}$$

is a bounded continuous map into L^1-maps of $\mathbb{R}$ into $S^1(H)$. Further

$$\begin{aligned} \int_{\mathbb{R}} \|t(x,x)\|_{S^1(H)} \,\mathrm{d}x &\leq \|T\|_{S^1(L^2(\mathbb{R},H))}, \\ \int_{\mathbb{R}} \mathrm{tr}_H(t(x,x)) \,\mathrm{d}x &= \mathrm{tr}_{L^2(\mathbb{R},H)}(T). \end{aligned} \tag{345}$$

If $[\partial, T]$ extends to trace-class, then (1) is continuous into the absolutely continuous L^1-maps: $\mathbb{R} \to S^1(H)$, and so T has a continuous kernel $t(x,y)$. Moreover

$$\|t(x,y)\|_{S^1(H)} \leq \|\partial T - \{T\partial\}\|_{S^1(L^2(\mathbb{R},H))}. \tag{346}$$

Remark 4.2. The kernel of an integral operator is defined only up to a set of measure zero in (x,y)-space, so (345) and (346) are meaningless unless the kernel is normalized in some way. The continuity of (344) normalizes t.

Especially Remark 4.2 to the Trace Lemma 4.1 is important to us. Our task is therefore to retrieve a kernel of the trace-class extensions of the operators $[\partial, P_t^+]$ and $[\partial, Q_t^+]$ with the desired continuity (344).

To that end, we need a method of constructing an $B(H)$-valued kernel with L^2-regularity first, which we will then manipulate to obtain kernels with the correct regularities in accordance with the Trace Lemma 4.1.

4.2 Construction of an operator valued integral kernel

Before we discuss the operators in $L^2(\mathbb{R}, H)$ from our setting, we will build an operator valued integral kernel for an abstract operator T in $L^2(\mathbb{R}, H)$. But first we note the following fundamental result concerning the relation of strong convergence and trace-class convergence (and cite it here as it is displayed in [16, Lemma 3.4]).

Lemma 4.3. *Let X be a separable, complex Hilbert space. Assume that R, R_n, T, $T_n \in B(X)$ are bounded operators for all $n \in \mathbb{N}$, such that for all $\phi \in X$ we have $\lim_{n\to\infty} \|(R_n - R)\phi\|_X = \lim_{n\to\infty} \|(T_n - T)\phi\|_X = 0$, and $S, S_n \in S^1(X)$ are trace-class operators for all $n \in \mathbb{N}$, such that $\lim_{n\to\infty} \|S_n - S\|_{S^1(X)} = 0$. Then*

$$\lim_{n\to\infty} \|R_n S_n T_n^* - RST^*\|_{S^1(X)} = 0. \tag{347}$$

As a consequence, we obtain the following Lemma 4.4, which will help us calculate the trace of an operator $\{[\partial, T]\}$, if it is trace-class.

Lemma 4.4. *Assume $\{[\partial, T]\}$ exists and is trace-class in $L^2(\mathbb{R}, H)$ for a bounded operator $T \in B\left(L^2(\mathbb{R}, H)\right)$. Then*

$$\operatorname{tr}_{L^2(\mathbb{R},H)}(\{[\partial, T]\}) = \lim_{\epsilon \searrow 0} \operatorname{tr}_{L^2(\mathbb{R},H)}\left(\left\{\left[\partial, e^{-\epsilon H_0} T e^{-\epsilon H_0}\right]\right\}\right). \tag{348}$$

Proof. By the functional calculus we have strong convergence of $e^{-\epsilon H_0}$ to 1 for $\epsilon \searrow 0$. Thus Lemma 4.3 implies that

$$\lim_{\epsilon \searrow 0} \left\|\{[\partial, T]\} - e^{-\epsilon H_0}\{[\partial, T]\} e^{-\epsilon H_0}\right\|_{S^1(L^2(\mathbb{R},H))} = 0. \tag{349}$$

Furthermore the operators ∂ and $e^{-\epsilon H_0}$ commute on the domain of ∂, therefore

$$e^{-\epsilon H_0}\{[\partial, T]\} e^{-\epsilon H_0} = \left\{\left[\partial, e^{-\epsilon H_0} T e^{-\epsilon H_0}\right]\right\}. \tag{350}$$

Since the trace is continuous with respect to the trace-norm, we conclude the statement (348) by combing (349) and (350). ∎

We thus introduce the following "mollified" auxiliary kernel k_T^ϵ, which has good regularity properties.

Proposition 4.5. *Let T be a bounded operator in $L^2(\mathbb{R}, H)$ and $\epsilon > 0$. Then*

$$k_T^\epsilon(x,y) := \left(H \ni \phi \mapsto \int_{\mathbb{R}} q_\epsilon(x-z) \left(e^{-\epsilon \widehat{A_-^2}} T \left(q_\epsilon(\cdot - y) \otimes e^{-\epsilon A_-^2} \phi \right) \right)(z)\, \mathrm{d}z \right), \quad (351)$$

where the integral is to be understood as a Bochner-integral in H, is well-defined as an element of $B(H)$ for all x, $y \in \mathbb{R}$, and

$$\begin{aligned} &k_T^\epsilon \in C_b^1\left(\mathbb{R}^2, B(H)\right), \\ &\|k_T^\epsilon\|_{C_b^1(\mathbb{R}^2, B(H))} \lesssim_\epsilon \|T\|_{B(L^2(\mathbb{R},H))}. \end{aligned} \quad (352)$$

Proof. We first note that for a fixed $\phi \in H$, the expression $e^{-\epsilon\widehat{A_-^2}} T\left(q_\epsilon(\cdot - y) \otimes e^{-\epsilon A_-^2}\phi\right)$ is an element of $L^2(\mathbb{R}, H)$, and thus, because $q_\epsilon(x - \cdot) \in L^2(\mathbb{R})$, the Bochner integral in (351) exists. It is also clear, that the right hand side of (351) is linear in the slot of ϕ. Furthermore, we may estimate for x, $y \in \mathbb{R}$ and $\phi \in H$:

$$\begin{aligned} \|k_T^\epsilon(x,y)\phi\|_H &\le \|q_\epsilon\|_{L^2(\mathbb{R})} \left\| e^{-\epsilon\widehat{A_-^2}} T\left(q_\epsilon(\cdot - y) \otimes e^{-\epsilon A_-^2}\phi\right)\right\|_{L^2(\mathbb{R},H)} \\ &\lesssim_\epsilon 1 \cdot \|T\|_{B(L^2(\mathbb{R},H))} \|q_\epsilon\|_{L^2(\mathbb{R})} \cdot 1 \cdot \|\phi\|_H \\ &\lesssim_\epsilon \|T\|_{B(L^2(\mathbb{R},H))} \|\phi\|_H, \end{aligned} \quad (353)$$

which shows for x, $y \in \mathbb{R}$, that $k_T^\epsilon(x,y) \in B(H)$.
We proceed by investigating the partial derivatives in x and y of $k_T^\epsilon(x,y)$ as a $B(H)$-valued function. Let x, $y \in \mathbb{R}$, $\delta > 0$ and, $h \neq 0$, $|h| \le \delta$. Then

$$\begin{aligned} &h^{-1} \Big\| k_T^\epsilon(x+h,y) - k_T^\epsilon(x,y) \\ &\quad -h \cdot \left(H \ni \phi \mapsto \int_{\mathbb{R}} q_\epsilon'(x-z) \left(e^{-\epsilon\widehat{A_-^2}} T\left(q_\epsilon(\cdot - y) \otimes e^{-\epsilon A_-^2}\phi\right)\right)(z)\,\mathrm{d}z \right) \Big\|_{B(H)} \\ \le & h^{-1} \sup_{\|\phi\|_H = 1} \left\| \left((\tau_h - id) q_\epsilon - h q_\epsilon' \right) *_{\mathbb{R}} \left(e^{-\epsilon\widehat{A_-^2}} T\left(q_\epsilon(\cdot - y) \otimes e^{-\epsilon A_-^2}\phi\right)\right)(x) \right\|_H \\ \le & h^{-1} \sup_{\|\phi\|_H = 1} \left\| (\tau_h - id) q_\epsilon - h q_\epsilon' \right\|_{L^2(\mathbb{R})} \|T\|_{B(L^2(\mathbb{R},H))} \|q_\epsilon\|_{L^2(\mathbb{R})} \|\phi\|_H \\ \lesssim_{\epsilon,T} & \left(\int_{\mathbb{R}} \left(h^{-1}\left(q_\epsilon(z+h) - q_\epsilon(z)\right) - q_\epsilon'(z) \right)^2 \mathrm{d}z \right)^{1/2} \end{aligned} \quad (354)$$

In the last line of (354) we wish to use Lebesgue's theorem of dominated convergence to conclude that the last expression goes to 0 as $h \to 0$. This is the case because by the mean value theorem the expression

$$2 \cdot \sup_{|w| \le \delta} \left(q_\epsilon'(z+w)\right)^2 + 2 \cdot \left(q_\epsilon'(z)\right)^2 \quad (355)$$

is an integrable dominant (independent of h). Similarly one deals with the partial derivative in y:

$$\begin{aligned}
&h^{-1} \| k_T^\epsilon (x, y+h) - k_T^\epsilon (x,y) \\
&\qquad -h \cdot \left(H \ni \phi \mapsto \int_{\mathbb{R}} q_\epsilon (x-z) \left(e^{-\epsilon \widehat{A_-^2}} T \left(-q_\epsilon' (\cdot - y) \otimes e^{-\epsilon A_-^2} \phi \right) \right) (z) \, \mathrm{d}z \right) \Bigg\|_{B(H)} \\
\le & h^{-1} \sup_{\|\phi\|_H = 1} \left\| \left(q_\epsilon *_{\mathbb{R}} \left(e^{-\epsilon \widehat{A_-^2}} T \left((\tau_h - id) q_\epsilon - h q_\epsilon' \right) (y - \cdot) \otimes e^{-\epsilon A_-^2} \phi \right) \right) (x) \right\|_H \\
\le & h^{-1} \sup_{\|\phi\|_H = 1} \|q_\epsilon\|_{L^2(\mathbb{R})} \|T\|_{B(L^2(\mathbb{R},H))} \left\| (\tau_h - id) q_\epsilon - h q_\epsilon' \right\|_{L^2(\mathbb{R})} \|\phi\|_H \\
\lesssim_{\epsilon, T} & \left(\int_{\mathbb{R}} \left(h^{-1} (q_\epsilon (z+h) - q_\epsilon (z)) - q_\epsilon' (z) \right)^2 \mathrm{d}z \right)^{1/2}, \qquad (356)
\end{aligned}$$

which goes to 0 as $h \to 0$ like before.
Next, we show the $B(H)$-norm-continuity of the partial derivatives, which we will do for the derivative in x. The derivative in y can be handled analogously. Let x, x', y, and $y' \in \mathbb{R}$.

$$\begin{aligned}
& \|\partial_1 k_T^\epsilon (x,y) - \partial_1 k_T^\epsilon (x,y)\|_{B(H)} \\
= & \sup_{\|\phi\|_H = 1} \Bigg\| \int_{\mathbb{R}} \left(q_\epsilon' (x-z) - q_\epsilon' (x'-z) \right) \left(e^{-\epsilon \widehat{A_-^2}} T \left(q_\epsilon (\cdot - y) \otimes e^{-\epsilon A_-^2} \phi \right) \right) (z) \, \mathrm{d}z \\
& \qquad + \int_{\mathbb{R}} q_\epsilon' (x'-z) \left(e^{-\epsilon \widehat{A_-^2}} T \left(\left(q_\epsilon (\cdot - y) - q_\epsilon (\cdot - y') \right) \otimes e^{-\epsilon A_-^2} \phi \right) \right) (z) \, \mathrm{d}z \Bigg\|_H \\
\le & \left\| (\tau_{x'-x} - id) q_\epsilon' \right\|_{L^2(\mathbb{R})} \|T\|_{B(L^2(\mathbb{R},H))} \|q_\epsilon\|_{L^2(\mathbb{R})} + \left\| q_\epsilon' \right\|_{L^2(\mathbb{R})} \|T\|_{B(L^2(\mathbb{R},H))} \left\| (\tau_{y'-y} - id) q_\epsilon' \right\|_{L^2(\mathbb{R})} \\
\lesssim_{\epsilon, T} & \left\| (\tau_{x'-x} - id) q_\epsilon' \right\|_{L^2(\mathbb{R})} + \left\| (\tau_{y'-y} - id) q_\epsilon' \right\|_{L^2(\mathbb{R})} \xrightarrow{(x,y) \to (x',y')} 0. \qquad (357)
\end{aligned}$$

In the last step, we used the strong continuity of the translation map τ. acting on $L^2(\mathbb{R})$. (Or one uses a suitable dominant and dominated convergence).
Thus, $k_T^\epsilon \in C^1 \left(\mathbb{R}^2, B(H) \right)$.
Finally we may estimate the norm of the derivative in x (and y analogously) in a similar manner as (353). For x, $y \in \mathbb{R}$ and $\phi \in H$ we find:

$$\begin{aligned}
\|\partial_1 k_T^\epsilon (x,y) \phi\|_H \le & \left\| q_\epsilon' \right\|_{L^2(\mathbb{R})} \left\| e^{-\epsilon \widehat{A_-^2}} T \left(q_\epsilon (\cdot - y) \otimes e^{-\epsilon A_-^2} \phi \right) \right\|_{L^2(\mathbb{R},H)} \\
\lesssim_\epsilon & 1 \cdot \|T\|_{B(L^2(\mathbb{R},H))} \|q_\epsilon\|_{L^2(\mathbb{R})} \cdot 1 \cdot \|\phi\|_H \\
\lesssim_\epsilon & \|T\|_{B(L^2(\mathbb{R},H))} \|\phi\|_H, \qquad (358)
\end{aligned}$$

which shows, together with (353), that

$$\|k_T^\epsilon\|_{C_b^1(\mathbb{R}^2, B(H))} \lesssim_\epsilon \|T\|_{B(L^2(\mathbb{R},H))}. \qquad (359)$$

■

The next step shows that the auxiliary kernel k_T^ϵ is indeed an integral kernel.

Lemma 4.6. *Let T be a bounded operator in $L^2(\mathbb{R}, H)$ and $\epsilon > 0$. Then the function k_T^ϵ, defined in Proposition 4.5, is an operator valued integral kernel of $e^{-\epsilon H_0} T e^{-\epsilon H_0}$, i.e. for $f \in C_c^\infty(\mathbb{R}, H)$ and a.e. $x \in \mathbb{R}$ we have*

$$\left(e^{-\epsilon H_0} T e^{-\epsilon H_0} f\right)(x) = \int_{\mathbb{R}} k_T^\epsilon(x, y) f(y) \,\mathrm{d}y. \tag{360}$$

Proof. Since $k_T^\epsilon \in C_b^1\left(\mathbb{R}^2, B(H)\right)$, by Proposition 4.5, we note that the right hand side of (360) is well-defined as a Bochner integral in H (c.f. Lemma 2.41). Since we seek equality in (360) almost everywhere, it certainly is sufficient to show equality in $L^2(\mathbb{R}, H)$. To that end, let $\rho, \eta \in C_c^\infty$ and $\phi, \psi \in H$, then, by Lemma 2.35, we conclude

$$\begin{aligned}
&\langle \eta \otimes \psi, e^{-\epsilon H_0} T e^{-\epsilon H_0} (\rho \otimes \phi) \rangle_{L^2(\mathbb{R}, H)} \\
=&\int_{\mathbb{R}} \langle \left(e^{-\epsilon H_0} (\eta \otimes \psi)\right)(z), \left(T e^{-\epsilon H_0} (\rho \otimes \phi)\right)(z) \rangle_H \mathrm{d}z \\
=&\int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}} \overline{\eta(w_1)} \rho(w_2) q_\epsilon(w_1 - z) \langle e^{-\epsilon A_-^2} \psi, \left(T\left(q_\epsilon(\cdot - w_2) \otimes e^{-\epsilon A_-^2} \phi\right)\right)(z) \rangle_H \mathrm{d}z \; \mathrm{d}w_2 \; \mathrm{d}w_1 \\
=&\langle \eta \otimes \psi, w_1 \mapsto \int_{\mathbb{R}} \int_{\mathbb{R}} q_\epsilon(w_1 - z) \left(\widehat{e^{-\epsilon A_-^2}} T\left(q_\epsilon(\cdot - w_2) \otimes e^{-\epsilon A_-^2} \phi\right)\right)(z) \,\mathrm{d}z \; \rho(w_2) \,\mathrm{d}w_2 \rangle_{L^2(\mathbb{R}, H)} \\
=&\langle \eta \otimes \psi, w_1 \mapsto \int_{\mathbb{R}} k_T^\epsilon(w_1, w_2) (\rho \otimes \phi)(w_2) \rangle_{L^2(\mathbb{R}, H)}.
\end{aligned} \tag{361}$$

By linearity, continuity and density we conclude that for $f, g \in L^2(\mathbb{R}, H)$ we obtain from (361) that

$$e^{-\epsilon H_0} T e^{-\epsilon H_0} f = x \mapsto \int_{\mathbb{R}} k_T^\epsilon(x, y) g(y) \,\mathrm{d}y, \tag{362}$$

where the equality holds in $L^2(\mathbb{R}, H)$, which finishes the proof. ∎

Since the kernel k_T^ϵ is differentiable in both arguments, we may consider the function $(\partial_1 + \partial_2) k_T^\epsilon$ as an integral kernel. Not surprising, this is a kernel of the commutator $\left\{\left[\partial, e^{-\epsilon H_0} T e^{-\epsilon H_0}\right]\right\}$.

Corollary 4.7. *Let T be a bounded operator in $L^2(\mathbb{R}, H)$ and $\epsilon > 0$. Then the function $(\partial_1 + \partial_2) k_T^\epsilon$, defined in Proposition 4.5, is an operator valued integral kernel of $\left\{\left[\partial, e^{-\epsilon H_0} T e^{-\epsilon H_0}\right]\right\}$, i.e. for $f \in C_c^\infty(\mathbb{R}, H)$ and a.e. $x \in \mathbb{R}$ we have*

$$\left(\left\{\left[\partial, e^{-\epsilon H_0} T e^{-\epsilon H_0}\right]\right\} f\right)(x) = \int_{\mathbb{R}} (\partial_1 + \partial_2) k_T^\epsilon(x, y) f(y) \,\mathrm{d}y. \tag{363}$$

Proof. We first note that $\left\{\left[\partial, e^{-\epsilon H_0} T e^{-\epsilon H_0}\right]\right\}$ indeed exists as a bounded operator in $L^2(\mathbb{R}, H)$, since $\left\{e^{-\epsilon H_0} \partial\right\}$ exists by Proposition 2.8 and Lemma 2.19. By equation (362) of Lemma 4.6 we find for $f, g \in C_c^\infty(\mathbb{R}, H)$

$$\langle \left\{\left[\partial, e^{-\epsilon H_0} T e^{-\epsilon H_0}\right]\right\} f, g \rangle_{L^2(\mathbb{R}, H)}$$

$$
\begin{aligned}
=&\langle e^{-\epsilon H_0} T e^{-\epsilon H_0} f', g\rangle_{L^2(\mathbb{R},H)} + \langle e^{-\epsilon H_0} T e^{-\epsilon H_0} f, g'\rangle_{L^2(\mathbb{R},H)} \\
=&\int_{\mathbb{R}}\int_{\mathbb{R}} \left(\langle k_T^\epsilon(x,y) f'(y), g(x)\rangle_H + \langle k_T^\epsilon(x,y) f(y), g'(x)\rangle_H\right) \mathrm{d}y\ \mathrm{d}x \\
=&\int_{\mathbb{R}}\int_{\mathbb{R}} \langle(\partial_1+\partial_2) k_T^\epsilon(x,y) f(y), g(x)\rangle_H\rangle_H \mathrm{d}y\ \mathrm{d}x \\
=&\langle x\mapsto \int_{\mathbb{R}} (\partial_1+\partial_2) k_T^\epsilon(x,y) f(y)\,\mathrm{d}y, g\rangle_{L^2(\mathbb{R},H)}.
\end{aligned} \tag{364}
$$

By continuity and density in (364) (recall that $k_T^\epsilon \in C_b^1\left(\mathbb{R}^2, B(H)\right)$ by Proposition 4.5), we conclude for $f \in L^2(\mathbb{R}, H)$

$$
x \mapsto \int_{\mathbb{R}} (\partial_1+\partial_2) k_T^\epsilon(x,y) f(y)\,\mathrm{d}y = \left\{\left[\partial, e^{-\epsilon H_0} T e^{-\epsilon H_0}\right]\right\} f, \tag{365}
$$

where the equality holds in $L^2(\mathbb{R}, H)$, thus finishing the proof. ∎

As we are equipped now with an integral kernel of "good regularity", we can compare it to the integral kernel one obtains from the Trace Lemma 4.1, given the correct trace-class membership.

Proposition 4.8. *Assume that for $\epsilon > 0$ the operator $e^{-\epsilon H_0} T e^{-\epsilon H_0}$ is trace-class in $L^2(\mathbb{R}, H)$. The function k_T^ϵ, defined in Proposition 4.5, then satisfies the following membership*

$$
h \mapsto \left(x \mapsto k_T^\epsilon(x, x+h)\right) \in C_b\left(L^1\left(\mathbb{R}, S^1(H)\right)\right). \tag{366}
$$

Proof. By the Trace Lemma 4.1 we know that there exists a operator valued integral kernel m_T^ϵ of $e^{-\epsilon H_0} T e^{-\epsilon H_0} \in S^1\left(L^2(\mathbb{R}, H)\right)$, such that

$$
h \mapsto \left(x \mapsto m_T^\epsilon(x, x+h)\right) \in C_b\left(\mathbb{R}, L^1\left(\mathbb{R}, S^1(H)\right)\right) \tag{367}
$$

and for all $f \in C_c^\infty(\mathbb{R}, H)$ and for a.e. $x \in \mathbb{R}$ we have

$$
\left(e^{-\epsilon H_0} T e^{-\epsilon H_0} f\right)(x) = \int_{\mathbb{R}} m_T^\epsilon(x,y) f(y)\,\mathrm{d}y. \tag{368}
$$

We wish to show that m_T^ϵ and k_T^ϵ coincide after embedding into a suitable space. To that end, let K be compact subset of $\mathbb{R}$ and consider the Banach space $C_b\left(\mathbb{R}, L^1(K, B(H))\right)$, endowed with the obvious norm. It is clear that the maps

$$
\begin{aligned}
i_1 :\ & C_b\left(\mathbb{R}^2, B(H)\right) \to C_b\left(\mathbb{R}, L^1(K, B(H))\right) \\
& f \mapsto \left(h \mapsto \left(x \mapsto f(x, x+h)\right)\right), \\
i_2 :\ & C_b\left(\mathbb{R}, L^1\left(\mathbb{R}, S^1(H)\right)\right) \to C_b\left(\mathbb{R}, L^1(K, B(H))\right) \\
& g \mapsto g,
\end{aligned} \tag{369}
$$

are well-defined, linear, and continuous. Let $Bil(X, Y)$ denote the space of continuous (bounded) bilinear forms of Banach spaces X and Y endowed with the norm

$$\|\phi\|_{Bil} := \sup_{x \in X, y \in Y} \frac{|\phi(x, y)|}{\|x\|_X \|y\|_Y}, \tag{370}$$

which turns $Bil(X, Y)$ into a Banach space.
We note that $C_c^\infty(\mathbb{R}) \otimes H$ is dense in $L^1(\mathbb{R}, H)$, since $C_c^\infty(\mathbb{R})$ is dense in $L^1(\mathbb{R})$ (via convolution with a mollifier), and because $L^1(\mathbb{R}) \otimes H$ is dense in $L^1(\mathbb{R}, H)$. We also note that $C(K) \otimes H$ is dense in $C(K, H)$ (c.f. also [35]).
Consider the map

$$\begin{aligned} (k \mapsto \phi_k) : C_b\left(\mathbb{R}, L^1(K, B(H))\right) &\to Bil\left(L^1(\mathbb{R}, H), C(K, H)\right) \\ \phi_k(f, g) &:= \int_K \int_{\mathbb{R}} \langle g(x), k(x, h) f(h) \rangle_H \mathrm{d}h \ \mathrm{d}x. \end{aligned} \tag{371}$$

The map $(k \mapsto \phi_k)$ is linear and continuous (bounded) because

$$\begin{aligned} \|\phi_k\|_{Bil(L^1(\mathbb{R},H), C(K,H))} &= \sup_{f \in L^1(\mathbb{R},H), g \in C(K,H)} \frac{\left|\int_K \int_{\mathbb{R}} \langle g(x), k(x,h) f(h) \rangle_H \mathrm{d}h \ \mathrm{d}x\right|}{\|f\|_{L^1(\mathbb{R},H)} \sup_{y \in K} \|g(y)\|_H} \\ &\leq \sup_{f \in L^1(\mathbb{R},H)} \frac{\int_K \int_{\mathbb{R}} \|k(x,h) f(h)\|_H \ \mathrm{d}h \ \mathrm{d}x}{\|f\|_{L^1(\mathbb{R},H)}} \\ &\leq \sup_{f \in L^1(\mathbb{R},H)} \frac{\int_{\mathbb{R}} \int_K \|k(x,h)\|_{B(H)} \ \mathrm{d}x \ \|f(h)\|_H \ \mathrm{d}x}{\|f\|_{L^1(\mathbb{R},H)}} \\ &\leq \sup_{h \in \mathbb{R}} \int_K \|k(x,h)\|_{B(H)} \ \mathrm{d}x. \end{aligned} \tag{372}$$

We claim that $(k \mapsto \phi_k)$ is injective.
Assume that there is $k \in C_b\left(\mathbb{R}, L^1(K, B(H))\right)$, such that for all $f \in L^1(\mathbb{R}, H)$ and $g \in C(K, H)$ the equality $\phi_k(f, g) = 0$ holds. Especially with $(e_n)_{n \in \mathbb{N}}$ denoting an orthonormal basis of H, we have, after using Fubini's theorem

$$\begin{aligned} &\forall n, m \in \mathbb{N},\ \xi \in C(K),\ \rho \in C_c^\infty(\mathbb{R}) : \\ &\phi_k(\rho \otimes e_n, \xi \otimes e_m) = \int_{\mathbb{R}} \rho(h) \int_K \langle \xi(x) e_m, k(x,h) e_n \rangle_H \mathrm{d}x \ \mathrm{d}h = 0. \end{aligned} \tag{373}$$

Since

$$h \mapsto \int_K \langle \xi(x) e_m, k(x,h) e_n \rangle_H \mathrm{d}x$$

is continuous (thus especially locally integrable) on $\mathbb{R}$, we conclude, by the principle of variation, that for all $h \in \mathbb{R}$ we have

$$\int_K \langle \xi(x) e_m, k(x,h) e_n \rangle_H \mathrm{d}x = 0. \tag{374}$$

Thus

$$\forall n,m\in\mathbb{N},\ \xi\in C\left(K\right),\ h\in\mathbb{R}:\int_{K}\overline{\xi\left(x\right)}\langle e_{m},k\left(x,h\right)e_{n}\rangle_{H}\mathrm{d}x=0. \tag{375}$$

Since for all $n,m\in\mathbb{N}$ and $h\in\mathbb{R}$ we have $\langle e_m,k\left(x,h\right)e_n\rangle_H\in L^1\left(\mathbb{R}\right)$, the principle of variation implies that for a.e. $x\in\mathbb{R}$, we have $\langle e_m,k\left(x,h\right)e_n\rangle_H=0$. Because $\mathbb{N}^2$ is countable and a countable union of null sets is still a null set, we may interchange the "for-a.e. quantor" over $x\in\mathbb{R}$ with the for-all quantor over $n,m\in\mathbb{N}$ in (375) and arrive at

$$\begin{aligned}&\forall h\in\mathbb{R}\text{ for a.e. }x\in\mathbb{R}\ \forall n,m\in\mathbb{N}:\langle e_{m},k\left(x,h\right)e_{n}\rangle_{H}=0.\\ \Rightarrow\ &\forall h\in\mathbb{R}\text{ for a.e. }x\in\mathbb{R}:k\left(x,h\right)=0\text{ in }B\left(H\right).\end{aligned} \tag{376}$$

This implies that $k\equiv0$ in $C_b\left(\mathbb{R},L^1\left(K,B\left(H\right)\right)\right)$, proving the injectivity of $\left(k\mapsto\phi_k\right)$. Define

$$\begin{aligned}k_1&:=i_1\left(k_T^{\epsilon}\right),\\ k_2&:=i_2\left(h\mapsto\left(x\mapsto m_T^{\epsilon}\left(x,x+h\right)\right)\right).\end{aligned} \tag{377}$$

Let $n,m\in\mathbb{N}$, $\rho\in C_c^{\infty}\left(\mathbb{R}\right)$ and $\xi\in C\left(K\right)$. Assume that $\operatorname{supp}\rho\subseteq K'$ for a compact subset $K'\subset\mathbb{R}$ and choose a compact interval $I\supseteq K+K'$. Define for an orthonormal basis $\left(e_n\right)_{n\in\mathbb{N}}$ of H

$$m_{l,n}^{\epsilon}\left(x,x+h\right):=\langle e_n,m_T^{\epsilon}\left(x,h\right)e_l\rangle_H.$$

Therefore

$$h\mapsto\left(x\mapsto m_{l,n}^{\epsilon}\left(x,x+h\right)\right)$$

is a function in $C_b\left(\mathbb{R},L^1\left(\mathbb{R}\right)\right)$. Note that for any compact set $K''\subset\mathbb{R}$ we additionally have

$$h\mapsto\left(x\mapsto m_{l,n}^{\epsilon}\left(x,x+h\right)\right)\in L^1\left(K''\times K\right), \tag{378}$$

for $\left(h,x\right)\in K''\times K$. Especially this holds for the compact set $K''=I-K'$. Then we have

$$\begin{aligned}\phi_{k_2}\left(\rho\otimes e_l,\xi\otimes e_n\right)&=\int_K\int_{\mathbb{R}}\rho\left(h\right)\overline{\xi\left(x\right)}m_{l,n}^{\epsilon}\left(x,x+h\right)\mathrm{d}h\ \mathrm{d}x\\ &=\int_{\left(x,y\right)\in K\times\mathbb{R}:y-x\in K''}\rho\left(y-x\right)\overline{\xi\left(x\right)}m_{l,n}^{\epsilon}\left(x,y\right)\mathrm{d}y\ \mathrm{d}x\\ &=\int_K\int_I\rho\left(y-x\right)\overline{\xi\left(x\right)}m_{l,n}^{\epsilon}\left(x,y\right)\mathrm{d}y\ \mathrm{d}x,\end{aligned} \tag{379}$$

where we note that $m_{l,n}^{\epsilon}\in L^1\left(K\times I\right)$, since

$$K\times I\subseteq\left\{\left(x,y\right)\in K\times\mathbb{R}:y-x\in K''\right\}. \tag{380}$$

Additionally, we note that we may approximate $(x,y) \mapsto \rho(y-x) \in C(K \times I)$ uniformly via

$$\rho(y-x) = \lim_{j\to\infty} \sum_{i=1}^{j} u_i^j(x) \rho\left(y - x_i^j\right), \tag{381}$$

where for $I =: [a,b]$ we set $x_i^j = a + \frac{(b-a)i}{j}$ and choose $u_i^j \in C^\infty(K)$ to form a partition of unity subordinated to the cover

$$U_i^j := K \cap \left(x_{i-1}^j - \frac{b-a}{3j}, x_i^j + \frac{b-a}{3j}\right). \tag{382}$$

Note that at most two partition functions have non-empty intersection of supports. The uniform convergence follows simply by noting that $\rho(y-x)$ is uniformly continuous on $K \times I$. Clearly

$$v_i^j := \rho\left(\cdot - x_i^j\right) \in C_c^\infty(\mathbb{R}), \tag{383}$$

and thus

$$\begin{aligned} &\int_K \int_I \rho(y-x) \overline{\xi(x)} m_{l,n}^\epsilon(x,y) \,\mathrm{d}y \,\mathrm{d}x \\ &= \int_K \int_I \left(\lim_{j\to\infty} \sum_{i=1}^{j} u_i^j(x) v_i^j(y) \right) \overline{\xi(x)} m_{l,n}^\epsilon(x,y) \,\mathrm{d}y \,\mathrm{d}x. \end{aligned} \tag{384}$$

Since

$$(x,y) \mapsto \overline{\xi(x)} m_{l,n}^\epsilon(x,y) \in L^1(K \times I), \tag{385}$$

and the sum (381) converges uniformly on $K \times I$, we conclude that the integrand of right hand side of (384) converges in $L^1(K \times I)$ and we are allowed to pull out the limit $j \to \infty$ and the (finite) sum. Since $v_i^j \otimes e_l \in C_c^\infty(\mathbb{R}, H)$ and $\xi \otimes e_n \in L^2(\mathbb{R}, H)$, by continuation with 0 outside K, we may combine (379), (384) and the above limit exchange consideration to conclude

$$\begin{aligned} \phi_{k_2}(\rho \otimes e_l, \xi \otimes e_n) &= \lim_{j\to\infty} \sum_{i=1}^{j} \int_K \int_I \langle \xi(x) e_n, m_T^\epsilon(x,y) \left(v_i^j(y) e_l\right) \rangle_H \mathrm{d}y \,\mathrm{d}x \\ &= \lim_{j\to\infty} \sum_{i=1}^{j} \langle \xi \otimes e_n e^{-\epsilon H_0} T e^{-\epsilon H_0} \left(v_i^j \otimes e_l\right) \rangle_{L^2(\mathbb{R},H)}. \end{aligned} \tag{386}$$

We note that

$$h \mapsto (x \mapsto \langle e_n, k_T^\epsilon(x,h) e_l \rangle_H)$$

is also an element of $L^1(K'' \times K)$ for any compact set $K'' \subset \mathbb{R}$, and we similarly obtain

$$\phi_{k_1}(\rho \otimes e_l, \xi \otimes e_n) = \lim_{j\to\infty} \sum_{i=1}^{j} \int_K \int_I \langle \xi(x) e_n, k_T^\epsilon(x,y) \left(v_i^j(y) e_l\right)\rangle_H \mathrm{d}y\, \mathrm{d}x$$
$$= \lim_{j\to\infty} \sum_{i=1}^{j} \langle \xi \otimes e_n, e^{-\epsilon H_0} T e^{-\epsilon H_0} \left(v_i^j \otimes e_l\right)\rangle_{L^2(\mathbb{R},H)}. \tag{387}$$

And thus, by density and continuity of $(k \mapsto \phi_k)$, we conclude $\phi_{k_1} = \phi_{k_2}$. The injectivity of $k \mapsto \phi_k$ then implies $k_1 = k_2$ as elements of $C_b\left(\mathbb{R}, L^1(K, B(H))\right)$ for any compact set $K \subset \mathbb{R}$. This implies that for each $h \in \mathbb{R}$ and a.e. $x \in K$ we have

$$k_T^\epsilon(x, x+h) = m_T^\epsilon(x, x+h) \in S^1(H), \tag{388}$$

by (367) and, since K was arbitrary, that

$$h \mapsto (x \mapsto k_T^\epsilon(x, x+h)) = h \mapsto (x \mapsto m_T^\epsilon(x, x+h)) \in C_b\left(\mathbb{R}, L^1\left(\mathbb{R}, S^1(H)\right)\right). \tag{389}$$

■

Again, we may also consider the commutator with ∂ and the corresponding integral kernel due to Corollary 4.7, giving us the analogous result and closing this subsection.

Corollary 4.9. *Let $\epsilon > 0$ and assume $\left\{\left[\partial, e^{-\epsilon H_0} T e^{-\epsilon H_0}\right]\right\}$ exists and is trace-class in $L^2(\mathbb{R}, H)$ for a bounded operator $T \in B\left(L^2(\mathbb{R}, H)\right)$. Then function k_T^ϵ, defined in Proposition 4.5, satisfies the following membership*

$$h \mapsto (x \mapsto (\partial_1 + \partial_2) k_T^\epsilon(x, x+h)) \in C_b\left(L^1\left(\mathbb{R}, S^1(H)\right)\right). \tag{390}$$

Proof. Since $\left\{\left[\partial, e^{-\epsilon H_0} T e^{-\epsilon H_0}\right]\right\}$ is trace class, there exists an operator valued integral kernel n_T^ϵ of $\left\{\left[\partial, e^{-\epsilon H_0} T e^{-\epsilon H_0}\right]\right\}$, such that

$$h \mapsto (x \mapsto n_t^\epsilon(x, x+h)) \in C_b\left(\mathbb{R}, L^1\left(\mathbb{R}, S^1(H)\right)\right), \tag{391}$$

according to the Trace Lemma 4.1. By Corollary 4.7, the $B(H)$-valued function $(\partial_1 + \partial_2) k_T^\epsilon \in C_b\left(\mathbb{R}^2, B(H)\right)$ is an operator valued integral kernel of $\left\{\left[\partial, e^{-\epsilon H_0} T e^{-\epsilon H_0}\right]\right\}$. Thus, analogous to the proof of Proposition 4.8, we show that $(\partial_1 + \partial_2) k_T^\epsilon$ must coincide in $C_b\left(\mathbb{R}, L^1(K, B(H))\right)$ with n_T^ϵ for each compact set $K \subset \mathbb{R}$, thus showing the membership

$$h \mapsto (x \mapsto (\partial_1 + \partial_2) k_T^\epsilon(x, x+h)) \in C_b\left(L^1\left(\mathbb{R}, S^1(H)\right)\right). \tag{392}$$

■

4.3 Calculation of the trace formulae

The previous subsection 4.2 gave us the needed tools to construct an integral kernel satisfying the normalization in the Trace Lemma 4.1. Thus we may calculate the trace of a commutator with ∂ by the following Theorem 4.10.

Theorem 4.10. *Assume $\{[\partial, T]\}$ exists and is trace-class in $L^2(\mathbb{R}, H)$ for a bounded operator $T \in B\left(L^2(\mathbb{R}, H)\right)$. Then for $\delta > 0$ we have*

$$\begin{aligned}
&\lim_{(y,y_0)\to(x,x_0)} k_T^\delta(x,x) - k_T^\delta(x_0,x_0) \in S^1(H), \text{ for } x, x_0 \in \mathbb{R}\cup\{\pm\infty\},\\
&\sup_{y,y_0\in\mathbb{R}} \left\| k_T^\delta(x,x) - k_T^\delta(x_0,x_0)\right\|_{S^1(H)} \leq \|\{[\partial,T]\}\|_{S^1(L^2(\mathbb{R},H))},\\
&\lim_{x\to x_0} \left\| k_T^\delta(x,x) - k_T^\delta(x_0,x_0)\right\|_{S^1(H)} = 0, \text{ for } x_0 \in \mathbb{R}\cup\{\pm\infty\},
\end{aligned} \tag{393}$$

where k^δ is defined in Proposition 4.5. Furthermore we have

$$\operatorname{tr}_{L^2(\mathbb{R},H)}(\{[\partial,T]\}) = \lim_{\epsilon\searrow 0} \operatorname{tr}_H\left(\lim_{(x_1,x_0)\to(+\infty,-\infty)} k_T^\epsilon(x_1,x_1) - k_T^\epsilon(x_0,x_0)\right). \tag{394}$$

Proof. By Proposition 4.8, we know that $(\partial_1 + \partial_2)\, k^\delta$ satisfies the normalization (344) of the Trace Lemma 4.1 pointed out in its Remark 4.2. Furthermore, $(\partial_1 + \partial_2)\, k^\delta$ is an operator valued integral kernel of $\left\{\left[\partial, e^{-\delta H_0} T e^{-\delta H_0}\right]\right\}$ by Corollary 4.7. Therefore, recalling equation (350), the Trace Lemma 4.1 enables us to conclude

$$\begin{aligned}
\int_{\mathbb{R}} \left\|(\partial_1+\partial_2)\, k^\delta(x,x)\right\|_{S^1(H)} \mathrm{d}x &\leq \left\|\left\{\left[\partial, e^{-\delta H_0} T e^{-\delta H_0}\right]\right\}\right\|_{S^1(L^2(\mathbb{R},H))}\\
&\leq \|\{[\partial,T]\}\|_{S^1(L^2(\mathbb{R},H))}.
\end{aligned} \tag{395}$$

Since also $k^\delta \in C_b^1\left(\mathbb{R}^2, B(H)\right)$, we have $\frac{\mathrm{d}}{\mathrm{d}x} k^\delta(x,x) = (\partial_1+\partial_2)\, k^\delta(x,x)$, and therefore for $x, x_0 \in \mathbb{R}$

$$k^\delta(x,x) - k^\delta(x_0,x_0) = \int_{x_0}^{x} (\partial_1+\partial_2)\, k^\delta(y,y)\, \mathrm{d}y \in S^1(H). \tag{396}$$

Furthermore, if $x, x_0 \in \mathbb{R}\cup\{\pm\infty\}$, by (396), the following limits exist in $S^1(H)$

$$\lim_{(y,y_0)\to(x,x_0)} k^\delta(x,x) - k^\delta(x_0,x_0) \in S^1(H). \tag{397}$$

Equation (396) and the estimate (395) then complete the proof of (393).
The Trace Lemma 4.1 additionally gives us the trace identity

$$\begin{aligned}
\operatorname{tr}_{L^2(\mathbb{R},H)}\left(\left\{\left[\partial, e^{-\epsilon H_0} T e^{-\epsilon H_0}\right]\right\}\right) &= \int_{\mathbb{R}} \operatorname{tr}_H\left((\partial_1+\partial_2)\, k_T^\epsilon(x,x)\right) \mathrm{d}x\\
= \operatorname{tr}_H\left(\int_{\mathbb{R}} (\partial_1+\partial_2)\, k_T^\epsilon(x,x)\, \mathrm{d}x\right) &= \operatorname{tr}_H\left(\lim_{(x_1,x_0)\to(+\infty,-\infty)} k_T^\epsilon(x_1,x_1) - k_T^\epsilon(x_0,x_0)\right),
\end{aligned} \tag{398}$$

and therefore, by Lemma 4.4, we obtain the trace identity (394). ■

The above Theorem 4.10 prompts us towards calculating the limits of the considered integral kernels at the ends of the diagonal. Since we know that these limits must exist in $S^1(H)$, it is enough to find the limits in a weaker topology.
If we return from an abstract operator T to our concrete setting, the following Proposition 4.11 is dedicated to determine the limits of the kernels $k^\epsilon_{P_t^+}$ and $k^\epsilon_{Q_t^+}$ at the ends of the diagonal in the weak operator topology of H. The proof will take some effort and we therefore inform the reader, that no details of the proof are used at some other point in this work.

Proposition 4.11. *Assume Hypothesis A2 (*2.11*) and either Hypothesis B1 (*2.12*) or B2 (*2.14*). Let $\epsilon, t > 0$ and $\phi, \psi \in H$. Define for $a, b > 0$ and $z \in \mathbb{C}$*

$$\chi_{a,b}(z) := \frac{e^{bz^2}}{2}\left(\operatorname{erf}\left((a+b)^{1/2} z\right) - \operatorname{erf}\left(b^{1/2} z\right)\right), \tag{399}$$

where erf *denotes the Gaussian error function.*
Then we obtain the following limits

$$\begin{aligned}
\lim_{x\to-\infty} \langle k^\epsilon_{P_t^+}(x,x)\phi, \psi\rangle_H &= (4\pi(t+2\epsilon))^{-1/2} \langle e^{-\epsilon A_-^2} A_- e^{-tA_-^2} e^{-\epsilon A_-^2}\phi, \psi\rangle_H, \\
\lim_{x\to+\infty} \langle k^\epsilon_{P_t^+}(x,x)\phi, \psi\rangle_H &= (4\pi(t+2\epsilon))^{-1/2} \langle e^{-\epsilon A_-^2} A_+ e^{-tA_+^2} e^{-\epsilon A_-^2}\phi, \psi\rangle_H, \\
\lim_{x\to-\infty} \langle k^\epsilon_{Q_t^+}(x,x)\phi, \psi\rangle_H &= t^{-1}\langle e^{-\epsilon A_-^2} \chi_{t,2\epsilon}(A_-) e^{-\epsilon A_-^2}\phi, \psi\rangle_H, \\
\lim_{x\to+\infty} \langle k^\epsilon_{Q_t^+}(x,x)\phi, \psi\rangle_H &= t^{-1}\langle e^{-\epsilon A_-^2} \chi_{t,2\epsilon}(A_+) e^{-\epsilon A_-^2}\phi, \psi\rangle_H.
\end{aligned} \tag{400}$$

Proof. Recall that the kernel k^ϵ_T from Proposition 4.5 is given by

$$k^\epsilon_T(x,y)\phi = \left(q_\epsilon *_{\mathbb{R}} \left(\widehat{e^{-\epsilon A_-^2}} T\left(q_\epsilon(\cdot - y)\otimes \phi\right)\right)\right)(x), \text{ for } x,\, y \in \mathbb{R} \text{ and } \phi \in H. \tag{401}$$

Denote for $x \in \mathbb{R}$ and $\phi \in H$

$$f^{\phi,x}_\epsilon := q_\epsilon(x - \cdot) \otimes \left(e^{-\epsilon A_-^2}\right)\phi \in L^2(\mathbb{R}, H). \tag{402}$$

One easily checks the identity

$$e^{-sH_0} f^{\phi,x}_\epsilon = f^{\phi,x}_{\epsilon+s}, \text{ for } x \in \mathbb{R},\ \phi \in H,\ \epsilon, s > 0. \tag{403}$$

Furthermore we have the estimates

$$\begin{aligned}
&\left\|D f^{\phi,x}_\epsilon\right\|_{L^2(\mathbb{R},H)} \\
&\le \left\|q'_\epsilon(x-\cdot)\otimes e^{-\epsilon A_-^2}\phi\right\|_{L^2(\mathbb{R},H)} + \left\|A(X)\,\widehat{e^{-\epsilon A_-^2}}\left(q_\epsilon(x-\cdot)\otimes\phi\right)\right\|_{L^2(\mathbb{R},H)} \lesssim_{\epsilon,\phi} 1, \\
&\left\|H_- f^{\phi,x}_\epsilon\right\|_{L^2(\mathbb{R},H)}
\end{aligned}$$

$$\leq \left\| q_\epsilon''(x-\cdot) \otimes e^{-\epsilon A_-^2}\phi \right\|_{L^2(\mathbb{R},H)} + \left\| \left(A(X)^2 - A'(X) \right) e^{-\epsilon \widehat{A_-^2}} \left(q_\epsilon(x-\cdot)\otimes\phi \right) \right\|_{L^2(\mathbb{R},H)}$$
$$\lesssim_{\epsilon,\phi} 1. \tag{404}$$

Therefore we have for $\phi, \psi \in H$ and $x \in \mathbb{R}$,

$$\begin{aligned} \langle k_T^\epsilon(x,x)\phi,\psi\rangle_H &= \int_{\mathbb{R}} q_\epsilon(x-z) \langle \left(e^{-\epsilon\widehat{A_-^2}} T \left(q_\epsilon(\cdot - x)\otimes e^{-\epsilon A_-^2}\phi \right) \right)(z), \psi\rangle_H \mathrm{d}z \\ &= \langle e^{-\epsilon \widehat{A_-^2}} T f_\epsilon^{\phi,x}, q_\epsilon(x-\cdot)\otimes\psi\rangle_{L^2(\mathbb{R},H)} \\ &= \langle T f_\epsilon^{\phi,x}, q_\epsilon(x-\cdot)\otimes e^{-\epsilon A_-^2}\psi\rangle_{L^2(\mathbb{R},H)} \\ &= \langle T f_\epsilon^{\phi,x}, f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)}. \end{aligned} \tag{405}$$

Thus if $T = P_t^+$, we have

$$\langle k_{P_t^+}^\epsilon(x,x)\phi,\psi\rangle_H = \langle e^{-tH_+} f_\epsilon^{\phi,x}, D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)}, \tag{406}$$

while for $T = Q_t^+$ we have

$$\begin{aligned} t\langle k_{Q_t^+}^\epsilon(x,x)\phi,\psi\rangle_H &= t\langle \gamma(tH_+) f_\epsilon^{\phi,x}, D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \\ &= \int_0^t \langle e^{-sH_+} f_\epsilon^{\phi,x}, D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \mathrm{d}s, \end{aligned} \tag{407}$$

by equation (321). We note further that (407) is the integral of (406), so if we calculate the limit of (406) in a uniform manner, we also obtain the limit of (407).
Note that

$$\begin{aligned} M_+ = H_+ - H_0 = DD^* - D_0 D_0^* &= D(D^* - D_0^*) + (D - D_0) D_0^* \\ &= D\left(A(X) - \widehat{A_-} \right) + \left(A(X) - \widehat{A_-} \right) D_0^*, \end{aligned} \tag{408}$$

which holds true on $\mathrm{Dom}(H_0)$. Combining (408) with Lemma 2.29 in (406), we obtain

$$\begin{aligned} &\langle e^{-tH_+} f_\epsilon^{\phi,x}, D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \\ =&\langle e^{-tH_0} f_\epsilon^{\phi,x}, D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} - \int_0^t \langle M_+ e^{-sH_0} f_\epsilon^{\phi,x}, e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \mathrm{d}s \\ =&\langle f_{\epsilon+t}^{\phi,x}, D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} - \int_0^t \langle \left(A(X) - \widehat{A_-} \right) f_{\epsilon+s}^{\phi,x}, D^* e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \mathrm{d}s \\ &- \int_0^t \langle D_0^* f_{\epsilon+s}^{\phi,x}, \left(A(X) - \widehat{A_-} \right) e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \mathrm{d}s. \end{aligned} \tag{409}$$

We have to discuss all three summands of the last line of (409).
Define

$$g_\epsilon(z) := \left\| e^{-\epsilon A_-^2} A'(z) e^{-\epsilon A_-^2} \right\|_{S^1(H)},$$

$$C_\epsilon := \int_{\mathbb{R}} g_\epsilon(z)\,\mathrm{d}z. \tag{410}$$

Let $\delta > 0$ and choose $R > 0$ large enough, such that

$$\begin{aligned}\int_{-\infty}^{-R} g_\epsilon(z)\,\mathrm{d}z &\le \delta,\\ (4\pi\epsilon)^{-1} C_\epsilon \int_R^\infty e^{-\frac{y^2}{2\epsilon}}\mathrm{d}y &\le \delta.\end{aligned} \tag{411}$$

For the first summand of the last line of (409) we obtain

$$\begin{aligned}&\langle f^{\phi,x}_{\epsilon+t}, Df^{\psi,x}_\epsilon\rangle_{L^2(\mathbb{R},H)}\\ =&\int_{\mathbb{R}} q_{\epsilon+t}(x-y)\,q_\epsilon(x-y)\,\langle e^{-(\epsilon+t)A_-^2}\phi, (A(y)-A_-)\,e^{-\epsilon A_-^2}\psi\rangle_H\mathrm{d}y\\ &+\int_{\mathbb{R}} q_{\epsilon+t}(x-y)\,q'_\epsilon(x-y)\,\langle e^{-(\epsilon+t)A_-^2}\phi, e^{-\epsilon A_-^2}\psi\rangle_H\mathrm{d}y\\ &+\int_{\mathbb{R}} q_{\epsilon+t}(x-y)\,q_\epsilon(x-y)\,\langle e^{-(\epsilon+t)A_-^2}\phi, A_-e^{-\epsilon A_-^2}\psi\rangle_H\mathrm{d}y\\ =&\int_{\mathbb{R}}\int_{-\infty}^y q_{\epsilon+t}(x-y)\,q_\epsilon(x-y)\,\langle\phi, e^{-(\epsilon+t)A_-^2}A'(z)\,e^{-\epsilon A_-^2}\psi\rangle_H\mathrm{d}z\ \mathrm{d}y\\ &+\int_{\mathbb{R}} q_{\epsilon+t}(x-y)\,q'_\epsilon(x-y)\,\mathrm{d}y\ \langle e^{-(\epsilon+t)A_-^2}\phi, e^{-\epsilon A_-^2}\psi\rangle_H\\ &+q_{2\epsilon+t}(0)\,\langle A_-e^{-(2\epsilon+t)A_-^2}\phi,\psi\rangle_H\\ =&\int_{\mathbb{R}}\int_{-\infty}^y q_{\epsilon+t}(x-y)\,q_\epsilon(x-y)\,\langle\phi, e^{-(\epsilon+t)A_-^2}A'(z)\,e^{-\epsilon A_-^2}\psi\rangle_H\mathrm{d}z\ \mathrm{d}y\\ &+0\\ &+(4\pi(2\epsilon+t))^{-1/2}\,\langle A_-e^{-(2\epsilon+t)A_-^2}\phi,\psi\rangle_H,\end{aligned} \tag{412}$$

where in the last step we used that $q_{\epsilon+t}$ is an even function, while q'_ϵ is odd, thus resulting in an integral of value 0. We estimate for $x \le -2R$

$$\begin{aligned}&\left|\langle f^{\phi,x}_{\epsilon+t}, Df^{\psi,x}_\epsilon\rangle_{L^2(\mathbb{R},H)} - (4\pi(2\epsilon+t))^{-1/2}\,\langle A_-e^{-(2\epsilon+t)A_-^2}\phi,\psi\rangle_H\right|\\ \le&\|\phi\|_H\,\|\psi\|_H\int_{\mathbb{R}}\left(\int_{-\infty}^y g_\epsilon(z)\,\mathrm{d}z\right)q_{\epsilon+t}(x-y)\,q_\epsilon(x-y)\,\mathrm{d}y\\ \le&\|\phi\|_H\,\|\psi\|_H\left(\int_{-\infty}^{-R}\left(\int_{-\infty}^{-R} g_\epsilon(z)\,\mathrm{d}z\right)q_{\epsilon+t}(x-y)\,q_\epsilon(x-y)\,\mathrm{d}y\right.\\ &\qquad\left.+\int_{\mathbb{R}} g_\epsilon(z)\,\mathrm{d}z\int_{-R}^\infty q_{\epsilon+t}(x-y)\,q_\epsilon(x-y)\,\mathrm{d}y\right)\\ &\lesssim_{\phi,\psi}\delta\cdot q_{2\epsilon+t}(0) + C_\epsilon\,(4\pi\epsilon)^{-1/2}\,(4\pi(\epsilon+t))^{-1/2}\int_R^\infty e^{-\frac{y^2}{2\epsilon}}\mathrm{d}y\\ &\lesssim_{\phi,\psi,\epsilon}\delta.\end{aligned} \tag{413}$$

By Lemma 2.40 we may rewrite the second summand of the last line of (409) by

$$\int_0^t \langle \left(A(X) - \widehat{A_-} \right) f_{\epsilon+s}^{\phi,x}, D^* e^{-(t-s)H_+} D f_\epsilon^{\psi,x} \rangle_{L^2(\mathbb{R},H)} \mathrm{d}s$$
$$= \int_0^t \langle \left(1 + \widehat{A_-^2}\right)^{-1/4} \left(A(X) - \widehat{A_-} \right) f_{\epsilon+s}^{\phi,x}, \left(1 + \widehat{A_-^2}\right)^{1/4} e^{-(t-s)H_-} H_- f_\epsilon^{\psi,x} \rangle_{L^2(\mathbb{R},H)} \mathrm{d}s$$
$$= \int_0^t \int_{\mathbb{R}} \langle \left(1 + A_-^2\right)^{-1/4} \left(A(y) - A_- \right) \left(1 + A_-^2\right)^{-3/4} \left(1 + A_-^2\right)^{3/4} e^{-(s+\epsilon)A_-^2} \phi \,,$$
$$\left(\left(1 + \widehat{A_-^2}\right)^{1/4} e^{-(t-s)H_-} H_- f_\epsilon^{\psi,x} \right)(y) \rangle_H q_{\epsilon+s}(x-y) \, \mathrm{d}y \, \mathrm{d}s \,. \tag{414}$$

By Lemma 3.3 there exists a function $g \in L^1(\mathbb{R})$ with

$$C := \|g\|_{L^1(\mathbb{R})} \,, \tag{415}$$

such that

$$\left\| \left(1 + A_-^2\right)^{-1/4} \left(A(y) - A_- \right) \left(1 + A_-^2\right)^{-3/4} \right\|_{S^1(H)} \leq G(y) := \int_{-\infty}^{y} |g(z)| \, \mathrm{d}z,$$
$$\left\| \left(1 + A_-^2\right)^{-1/4} \left(A_+ - A(y) \right) \left(1 + A_-^2\right)^{-3/4} \right\|_{S^1(H)} \leq \widetilde{G}(y) := \int_{y}^{+\infty} |g(z)| \, \mathrm{d}z. \tag{416}$$

For $t_0 > 0$ let $\delta > 0$ and choose $r > 0$ large enough, such that

$$\int_{-\infty}^{-r} |g(z)| \, \mathrm{d}z + \int_{r}^{+\infty} |g(z)| \, \mathrm{d}z \leq \delta,$$
$$\left((4\pi\epsilon)^{-1} \int_r^{+\infty} \left(1 + \frac{|z|}{2\epsilon} \right)^2 e^{-\frac{z^2}{2(t_0+\epsilon)}} \mathrm{d}z \right)^{1/2} \leq \delta. \tag{417}$$

Corollary 2.39, Lemma 2.36, estimate (404), and (416) imply that we may estimate (414) for $0 < s < t \leq t_0$ and $x \leq -2r$ by

$$\left| \int_0^t \langle \left(A(X) - \widehat{A_-} \right) f_{\epsilon+s}^{\phi,x}, D^* e^{-(t-s)H_+} D f_\epsilon^{\psi,x} \rangle_{L^2(\mathbb{R},H)} \mathrm{d}s \right|$$
$$\lesssim_{t_0} \|\phi\|_H \int_0^t \int_{\mathbb{R}} G(y) (s+\epsilon)^{-3/4} q_{\epsilon+s}(x-y)$$
$$\left\| \left(\left(1 + \widehat{A_-^2}\right)^{1/4} e^{-(t-s)H_-} H_- f_\epsilon^{\psi,x} \right)(y) \right\|_H \mathrm{d}y \, \mathrm{d}s$$
$$\lesssim_{t_0,\epsilon,\phi} \int_0^t \int_{-\infty}^{-r} \int_{-\infty}^{y} g(z) \, \mathrm{d}z \; q_{\epsilon+s}(x-y) \left\| \left(\left(1 + \widehat{A_-^2}\right)^{1/4} e^{-(t-s)H_-} H_- f_\epsilon^{\psi,x} \right)(y) \right\|_H \mathrm{d}y \, \mathrm{d}s$$
$$+ \int_0^t \int_{-r}^{+\infty} \int_{\mathbb{R}} g(z) \, \mathrm{d}z \; q_{\epsilon+s}(x-y) \left\| \left(\left(1 + \widehat{A_-^2}\right)^{1/4} e^{-(t-s)H_-} H_- f_\epsilon^{\psi,x} \right)(y) \right\|_H \mathrm{d}y \, \mathrm{d}s$$
$$\lesssim_{t_0,\epsilon,\phi} \delta \int_0^t \|q_{s+\epsilon}\|_{L^2(\mathbb{R})} \left\| \left(1 + \widehat{A_-^2}\right)^{1/4} e^{-(t-s)H_-} H_- f_\epsilon^{\psi,x} \right\|_{L^2(\mathbb{R},H)} \mathrm{d}s$$

$$+ C\int_0^t \|q_{s+\epsilon}(x-\cdot)\|_{L^2((-r,+\infty))} \left\|\left(1+\widehat{A_-^2}\right)^{1/4} e^{-(t-s)H_-} H_- f_\epsilon^{\psi,x}\right\|_{L^2(\mathbb{R},H)} \mathrm{d}s$$

$$\lesssim_{t_0,\epsilon,\phi,\psi} \delta\int_0^t (s+\epsilon)^{-1/4}(t-s)^{-1/4}\,\mathrm{d}s$$

$$+\int_0^t \left(\int_r^{+\infty} q_{s+\epsilon}(z)^2\,\mathrm{d}z\right)^{1/2}(t-s)^{-1/4}\,\mathrm{d}s$$

$$\lesssim_{t_0,\epsilon,\phi,\psi} \delta t^{3/4} + \int_0^t\left((4\pi\epsilon)^{-1}\int_r^{+\infty} e^{-\frac{z^2}{2(t_0+\epsilon)}}\mathrm{d}z\right)^{1/2}(t-s)^{-1/4}\,\mathrm{d}s$$

$$\lesssim_{t_0,\epsilon,\phi,\psi} \delta t^{3/4} + \delta t^{3/4}. \tag{418}$$

For the remaining third summand of the last line of (409) we find

$$\int_0^t \langle D_0^* f_{\epsilon+s}^{\phi,x}, \left(A(X)-\widehat{A_-}\right) e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)}\mathrm{d}s$$

$$= \int_0^t \langle -\partial\left(1+\widehat{A_-^2}\right)^{1/4} f_{\epsilon+s}^{\phi,x}, \left(1+\widehat{A_-^2}\right)^{-1/4}\left(A(X)-\widehat{A_-}\right) e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)}\mathrm{d}s$$

$$+ \int_0^t \langle \widehat{A_-}\left(1+\widehat{A_-^2}\right)^{1/4} f_{\epsilon+s}^{\phi,x}, \left(1+\widehat{A_-^2}\right)^{-1/4}\left(A(X)-\widehat{A_-}\right) e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)}\mathrm{d}s$$

$$= \int_0^t\int_{\mathbb{R}} \langle \left(1+A_-^2\right)^{1/4} e^{-(s+\epsilon)A_-^2}\phi, \left(1+A_-^2\right)^{-1/4}\left(A(y)-A_-\right)\left(1+A_-^2\right)^{-3/4}$$

$$\left(\left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\right)(y)\rangle_H q_{s+\epsilon}'(x-y)\,\mathrm{d}y\ \mathrm{d}s$$

$$+ \int_0^t\int_{\mathbb{R}} \langle A_-\left(1+A_-^2\right)^{1/4} e^{-(s+\epsilon)A_-^2}\phi, \left(1+A_-^2\right)^{-1/4}\left(A(y)-A_-\right)\left(1+A_-^2\right)^{-3/4}$$

$$\left(\left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\right)(y)\rangle_H q_{s+\epsilon}(x-y)\,\mathrm{d}y\ \mathrm{d}s\ . \tag{419}$$

Corollary 2.39, Lemma 2.36, estimate (404) and (416) imply that we may estimate (419) for $0 < s < t \leq t_0$ and $x \leq -2r$ by

$$\left|\int_0^t \langle D_0^* f_{\epsilon+s}^{\phi,x}, \left(A(X)-\widehat{A_-}\right) e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)}\mathrm{d}s\right|$$

$$\lesssim_{t_0} \|\phi\|_H \int_0^t\int_{\mathbb{R}} G(y)(s+\epsilon)^{-1/4}\left|q_{\epsilon+s}'(x-y)\right|$$

$$\left\|\left(\left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\right)(y)\right\|_H \mathrm{d}y\ \mathrm{d}s$$

$$+ \|\phi\|_H \int_0^t\int_{\mathbb{R}} G(y)(s+\epsilon)^{-3/4} q_{\epsilon+s}(x-y)$$

$$\left\|\left(\left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\right)(y)\right\|_H \mathrm{d}y\ \mathrm{d}s$$

$$
\begin{aligned}
&\lesssim_{t_0,\epsilon,\phi} \int_0^t \int_{-\infty}^{-r} \int_{-\infty}^{y} g(z)\,\mathrm{d}z \left|q'_{\epsilon+s}(x-y)\right| \left\| \left(\left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x} \right)(y) \right\|_H \mathrm{d}y\ \mathrm{d}s \\
&\quad + \int_0^t \int_{-r}^{+\infty} \int_{\mathbb{R}} g(z)\,\mathrm{d}z \left|q'_{\epsilon+s}(x-y)\right| \left\| \left(\left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x} \right)(y) \right\|_H \mathrm{d}y\ \mathrm{d}s \\
&\quad + \int_0^t \int_{-\infty}^{-r} \int_{-\infty}^{y} g(z)\,\mathrm{d}z\ q_{\epsilon+s}(x-y) \left\| \left(\left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x} \right)(y) \right\|_H \mathrm{d}y\ \mathrm{d}s \\
&\quad + \int_0^t \int_{-r}^{+\infty} \int_{\mathbb{R}} g(z)\,\mathrm{d}z\ q_{\epsilon+s}(x-y) \left\| \left(\left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x} \right)(y) \right\|_H \mathrm{d}y\ \mathrm{d}s \\
&\lesssim_{t_0,\epsilon,\phi} \delta \int_0^t \left\| \left|q'_{s+\epsilon}\right| + q_{s+\epsilon} \right\|_{L^2(\mathbb{R})} \left\| \left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x} \right\|_{L^2(\mathbb{R},H)} \mathrm{d}s \\
&\quad + C \int_0^t \left\| \left|q'_{s+\epsilon}(x-\cdot)\right| + q_{s+\epsilon}(x-\cdot) \right\|_{L^2((-r,+\infty))} \\
&\qquad\qquad \left\| \left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x} \right\|_{L^2(\mathbb{R},H)} \mathrm{d}s \\
&\lesssim_{t_0,\epsilon,\phi,\psi} \delta \int_0^t \left((s+\epsilon)^{-3/4} + (s+\epsilon)^{-1/4} \right) (t-s)^{-3/4} \mathrm{d}s \\
&\quad + \int_0^t \left(\int_r^{+\infty} \left(\left|q'_{s+\epsilon}(z)\right| + q_{s+\epsilon}(z) \right)^2 \mathrm{d}z \right)^{1/2} (t-s)^{-3/4} \mathrm{d}s \\
&\lesssim_{t_0,\epsilon,\phi,\psi} \delta t^{1/4} + \int_0^t \left((4\pi\epsilon)^{-1} \int_r^{+\infty} \left(1+\frac{|z|}{2\epsilon}\right)^2 e^{-\frac{z^2}{2(t_0+\epsilon)}} \mathrm{d}z \right)^{1/2} (t-s)^{-3/4} \mathrm{d}s \\
&\lesssim_{t_0,\epsilon,\phi,\psi} \delta t^{1/4} + \delta t^{1/4}.
\end{aligned} \tag{420}
$$

Compiling the estimates (413), (418) and (420), we obtain by (406) and (409) for $0 < t \leq t_0$ and $x \leq 2\min(r, R)$

$$
\begin{aligned}
&\left| \langle k^\epsilon_{P_t^+}(x,x)\,\phi, \psi \rangle_{L^2(\mathbb{R},H)} - (4\pi(2\epsilon+t))^{-1/2} \langle A_- e^{-(t+2\epsilon)A_-^2} \phi, \psi \rangle_H \right| \\
&\lesssim_{t_0,\epsilon,\phi,\psi} \delta \left(1 + t^{1/4} + t^{3/4}\right).
\end{aligned} \tag{421}
$$

And by (407) we obtain

$$
\begin{aligned}
&\left| t \langle k^\epsilon_{Q_t^+}(x,x)\,\phi, \psi \rangle_{L^2(\mathbb{R},H)} - \int_0^t (4\pi(2\epsilon+s))^{-1/2} \langle A_- e^{-(2\epsilon+s)A_-^2} \phi, \psi \rangle_H \mathrm{d}s \right| \\
&\lesssim_{t_0,\epsilon,\phi,\psi} \int_0^t \delta \left(1 + s^{1/4} + s^{3/4}\right) \mathrm{d}s \lesssim_{t_0,\epsilon,\phi,\psi,t} \delta.
\end{aligned} \tag{422}
$$

Since $\delta > 0$ was arbitrary we conclude from (421)

$$
\lim_{x\to-\infty} \langle k^\epsilon_{P_t^+}(x,x)\,\phi, \psi \rangle_H = (4\pi(t+2\epsilon))^{-1/2} \langle A_- e^{-(t+2\epsilon)A_-^2} \phi, \psi \rangle_H, \tag{423}
$$

and from (422)

$$
\lim_{x\to-\infty} \langle k^\epsilon_{Q_t^+}(x,x)\,\phi, \psi \rangle_H = t^{-1} \int_0^t (4\pi(s+2\epsilon))^{-1/2} \langle A_- e^{-(s+2\epsilon)A_-^2} \phi, \psi \rangle_H \mathrm{d}s, \tag{424}
$$

Integration by substitution yields

$$\int_0^t (4\pi (s+2\epsilon))^{-1/2} z e^{-(s+2\epsilon)z^2} \mathrm{d}s = \frac{1}{2}\left(\operatorname{erf}\left((t+2\epsilon)^{1/2} z\right) - \operatorname{erf}\left((2\epsilon)^{1/2} z\right)\right)$$
$$= e^{-2\epsilon z^2} \chi_{t,2\epsilon}(z). \tag{425}$$

Note also that $\chi_{a,b}$ is a bounded function on $\mathbb{R}$ for $a, b > 0$, and thus $\chi_{t,2\epsilon}(A_\pm)$ are bounded operators in H. Therefore (424) can be restated as

$$\lim_{x\to-\infty} \langle k^{\epsilon}_{Q_t^+}(x,x)\phi, \psi\rangle_H = t^{-1} \langle e^{-\epsilon A_-^2} \chi_{t,2\epsilon}(A_-) e^{-\epsilon A_-^2} \phi, \psi\rangle_H. \tag{426}$$

Next, let us discuss the limits for $x \to +\infty$. Most of the calculations done for $x \to -\infty$ carry over and we can argue by analogy, however one has to be careful and consider in which terms one replaces A_- by A_+ and in which one does not. We will therefore discuss the needed amendments.

We first introduce the operator $D_1 := \partial + \widehat{A_+}$, which has the same properties as the operator D_0. In particular, by Lemma 2.24, we find analogous to Lemma 2.6, that $\mathrm{Dom}(D_1)_\Gamma = H^1(\mathbb{R}, H) \cap L^2(\mathbb{R}, \mathrm{Dom}(A_-)_\Gamma)$ and that $D_1^* = -\partial + \widehat{A_+}$ with $\mathrm{Dom}(D_1^*) = \mathrm{Dom}(D_1) = \mathrm{Dom}(D_0)$. Introducing $H_1 := D_1^* D_1$, we note that $H_1 \geq 0$ is self-adjoint in $L^2(\mathbb{R}, H)$ and $H_1 = -\partial^2 + \widehat{A_+^2}$ holds, analogous to Lemma 2.8. Lemma 2.24 then implies that $\mathrm{Dom}(H_1)_\Gamma = \mathrm{Dom}(H_0)_\Gamma$.

Therefore, also the analogy of Lemma 2.29 for H_1 holds true, i.e. for $t_0 \geq t > 0$ we have

$$e^{-tH_\pm} - e^{-tH_1} = -\int_0^t e^{-sH_\pm} N_\pm e^{-(t-s)H_1} \mathrm{d}s$$
$$= -\int_0^t e^{-sH_0} N_\pm e^{-(t-s)H_\pm} \mathrm{d}s, \tag{427}$$

where the integrals converge in $B\left(L^2(\mathbb{R}, H)\right)$-norm and $N_\pm := A(X)^2 - \widehat{A_+^2} \pm A'(X)$. We replace (408) by

$$N_+ = D\left(A(X) - \widehat{A_+}\right) + \left(A(X) - \widehat{A_+}\right) D_1^*, \tag{428}$$

which holds true on $\mathrm{Dom}(H_1) = \mathrm{Dom}(H_0)$. Combining (428) with (427) in (406), we obtain

$$\begin{aligned}
&\langle e^{-tH_+} f_\epsilon^{\phi,x}, D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \\
=&\langle e^{-tH_1} f_\epsilon^{\phi,x}, D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} - \int_0^t \langle N_+ e^{-sH_1} f_\epsilon^{\phi,x}, e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \mathrm{d}s \\
=&\langle e^{-tH_1} f_\epsilon^{\phi,x}, D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \\
&- \int_0^t \langle \left(A(X) - \widehat{A_+}\right) e^{-sH_1} f_\epsilon^{\phi,x}, D^* e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \mathrm{d}s \\
&- \int_0^t \langle D_1^* e^{-sH_1} f_\epsilon^{\phi,x}, \left(A(X) - \widehat{A_+}\right) e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \mathrm{d}s.
\end{aligned} \tag{429}$$

Analogous to (412) we obtain for the first summand of the last line of (429)

$$
\begin{aligned}
&\langle e^{-tH_1} f_\epsilon^{\phi,x}, D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \\
=& \int_{\mathbb{R}} q_{\epsilon+t}(x-y)\, q_\epsilon(x-y) \\
&\quad \langle \phi, e^{-\epsilon A_-^2} e^{-tA_+^2} \left(1+A_-^2\right)^{1/4} \left(1+A_-^2\right)^{-1/4} \left(A(y)-A_+\right) e^{-\epsilon A_-^2}\psi\rangle_H \mathrm{d}y \\
&+0 \\
&+ \left(4\pi\left(2\epsilon+t\right)\right)^{-1/2} \langle e^{-\epsilon A_-^2} A_+ e^{-tA_+^2} e^{-\epsilon A_-^2}\phi, \psi\rangle_H. \qquad (430)
\end{aligned}
$$

Let $\delta > 0$ and choose $R > 0$ large enough, such that

$$
\widetilde{G}(R) \leq \delta, \ \int_{-\infty}^{-R} e^{-\frac{y^2}{2\epsilon}} \mathrm{d}y \leq \delta. \qquad (431)
$$

Then for $t_0 \geq t > 0$ and $x \geq 2R$ we estimate, using (416) in (430)

$$
\begin{aligned}
&\left| \langle e^{-tH_1} f_\epsilon^{\phi,x}, D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} - \left(4\pi\left(2\epsilon+t\right)\right)^{-1/2} \langle e^{-\epsilon A_-^2} A_+ e^{-tA_+^2} e^{-\epsilon A_-^2}\phi, \psi\rangle_H \right| \\
\lesssim_{\phi,\psi,t_0,\epsilon}& \int_{\mathbb{R}} q_{\epsilon+t}(x-y)\, q_\epsilon(x-y)\, t^{-1/4} \widetilde{G}(y)\, \mathrm{d}y \\
\lesssim_{\phi,\psi,t_0,\epsilon}& t^{-1/4} \int_R^{+\infty} \widetilde{G}(R)\, q_{\epsilon+t}(x-y)\, q_\epsilon(x-y)\, \mathrm{d}y \\
&+ t^{-1/4} \int_{-\infty}^{R} \left(\int_{\mathbb{R}} g(z)\, \mathrm{d}z \right) q_{\epsilon+t}(x-y)\, q_\epsilon(x-y)\, \mathrm{d}y \\
\lesssim_{\phi,\psi,t_0,\epsilon}& t^{-1/4} \left(\delta + \|g\|_{L^1(\mathbb{R})} \left(4\pi\epsilon\right)^{-1/2} \left(4\pi t\right)^{-1/2} \int_{-\infty}^{-R} e^{-\frac{y^2}{2\epsilon}} \mathrm{d}y \right) \\
\lesssim_{\phi,\psi,t_0,\epsilon}& \delta t^{-1/4}. \qquad (432)
\end{aligned}
$$

For the second summand of the last line of (429) we find for $t_0 \geq t > 0$ and $x \geq 2r$ by (417)

$$
\begin{aligned}
&\left| \int_0^t \langle \left(A(X) - \widehat{A_+}\right) e^{-sH_1} f_\epsilon^{\phi,x}, D^* e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \mathrm{d}s \right| \\
\lesssim_{t_0,\epsilon,\phi}& \int_0^t \int_{\mathbb{R}} \widetilde{G}(y)\, s^{-3/4} q_{\epsilon+s}(x-y) \left\| \left(\left(1+\widehat{A_-^2}\right)^{1/4} e^{-(t-s)H_-} H_- f_\epsilon^{\psi,x} \right)(y) \right\|_H \mathrm{d}y\ \mathrm{d}s \\
\lesssim_{t_0,\epsilon,\phi}& \delta \int_0^t s^{-3/4} \|q_{\epsilon+s}\|_{L^2(\mathbb{R},H)} \left\| \left(1+\widehat{A_-^2}\right)^{1/4} e^{-(t-s)H_-} H_- f_\epsilon^{\psi,x} \right\|_{L^2(\mathbb{R},H)} \mathrm{d}s \\
&+ C \int_0^t s^{-3/4} \|q_{s+\epsilon}(x-\cdot)\|_{L^2((-\infty,r))} \left\| \left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_-} H_- f_\epsilon^{\psi,x} \right\|_{L^2(\mathbb{R},H)} \mathrm{d}s \\
\lesssim_{t_0,\epsilon,\phi,\psi}& \delta \int_0^t s^{-3/4} (t-s)^{-1/4} \mathrm{d}s + \int_0^t s^{-3/4} \left(\int_r^{+\infty} q_{s+\epsilon}(z)^2 \mathrm{d}z \right)^{1/2} (t-s)^{-1/4} \mathrm{d}s \\
\lesssim_{t_0,\epsilon,\phi,\psi}& \delta. \qquad (433)
\end{aligned}
$$

Lastly for the third summand of the last line of (429) we find for $t_0 \geq t > 0$ and $x \geq 2r$ by (417)

$$\begin{aligned}
&\left|\int_0^t \langle D_1^* e^{-sH_1} f_\epsilon^{\phi,x}, \left(A(X) - \widehat{A_+}\right) e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \mathrm{d}s\right| \\
&\leq \left|\int_0^t \langle -\partial \left(1+\widehat{A_-^2}\right)^{1/4} e^{-sH_1} f_\epsilon^{\phi,x}, \left(1+\widehat{A_-^2}\right)^{-1/4} \left(A(X) - \widehat{A_+}\right) \left(1+\widehat{A_-^2}\right)^{-3/4}\right. \\
&\qquad\left. \left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \mathrm{d}s\right| \\
&\quad + \left|\int_0^t \langle \widehat{A_+} \left(1+\widehat{A_+^2}\right)^{1/4} e^{-sH_1} f_\epsilon^{\phi,x}, \left(1+\widehat{A_+^2}\right)^{-1/4} \left(1+\widehat{A_-^2}\right)^{1/4} \left(1+\widehat{A_-^2}\right)^{-1/4}\right. \\
&\qquad\left. \left(A(X) - \widehat{A_+}\right) \left(1+\widehat{A_-^2}\right)^{-3/4} \left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\rangle_{L^2(\mathbb{R},H)} \mathrm{d}s\right| \\
&\lesssim_{t_0,\epsilon,\phi} \int_0^t \int_{\mathbb{R}} \widetilde{G}(y) s^{-1/4} \left|q'_{\epsilon+s}(x-y)\right| \left\|\left(\left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\right)(y)\right\|_H \mathrm{d}y\ \mathrm{d}s \\
&\quad + \int_0^t \int_{\mathbb{R}} \widetilde{G}(y) s^{-3/4} q_{\epsilon+s}(x-y) \left\|\left(\left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\right)(y)\right\|_H \mathrm{d}y\ \mathrm{d}s \\
&\lesssim_{t_0,\epsilon,\phi} \delta \int_0^t \left\|s^{-1/4}\left|q'_{s+\epsilon}\right| + s^{-3/4} q_{s+\epsilon}\right\|_{L^2(\mathbb{R})} \left\|\left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\right\|_{L^2(\mathbb{R},H)} \mathrm{d}s \\
&\quad + C \int_0^t \left\|s^{-1/4}\left|q'_{s+\epsilon}\right| + s^{-3/4} q_{s+\epsilon}\right\|_{L^2((-\infty,r))} \\
&\qquad \left\|\left(1+\widehat{A_-^2}\right)^{3/4} e^{-(t-s)H_+} D f_\epsilon^{\psi,x}\right\|_{L^2(\mathbb{R},H)} \mathrm{d}s \\
&\lesssim_{t_0,\epsilon,\phi,\psi} \delta \int_0^t \left(s^{-1/4}(s+\epsilon)^{-3/4} + s^{-3/4}(s+\epsilon)^{-1/4}\right)(t-s)^{-3/4} \mathrm{d}s \\
&\quad + \int_0^t \left(s^{-1/4} + s^{-3/4}\right) \left((4\pi\epsilon)^{-1} \int_{-\infty}^r \left(1+\frac{|z|}{2\epsilon}\right)^2 e^{-\frac{z^2}{2(t_0+\epsilon)}} \mathrm{d}z\right)^{1/2} (t-s)^{-3/4} \mathrm{d}s \\
&\lesssim_{t_0,\epsilon,\phi,\psi} \delta t^{-1/2} + \delta t^{-1/2}.
\end{aligned} \tag{434}$$

Compiling the estimates (432), (433) and (434), we obtain by (406) and (429) for $0 < t \leq t_0$ and $x \geq 2\min(r,R)$

$$\begin{aligned}
&\left|\langle k^\epsilon_{P_t^+}(x,x)\phi,\psi\rangle_{L^2(\mathbb{R},H)} - (4\pi(2\epsilon+t))^{-1/2} \langle e^{-\epsilon A_-^2} A_+ e^{-tA_+^2} e^{-\epsilon A_-^2}\phi,\psi\rangle_H\right| \\
&\lesssim_{t_0,\epsilon,\phi,\psi} \delta\left(1 + t^{-1/4} + t^{-1/2}\right).
\end{aligned} \tag{435}$$

And by (407) we obtain

$$\begin{aligned}
&\left|t\langle k^\epsilon_{Q_t^+}(x,x)\phi,\psi\rangle_{L^2(\mathbb{R},H)} - \int_0^t (4\pi(2\epsilon+s))^{-1/2} \langle e^{-\epsilon A_-^2} A_+ e^{-tA_+^2} e^{-\epsilon A_-^2}\phi,\psi\rangle_H \mathrm{d}s\right| \\
&\lesssim_{t_0,\epsilon,\phi,\psi} \int_0^t \delta\left(1 + s^{-1/4} + s^{-1/2}\right) \mathrm{d}s \lesssim_{t_0,\epsilon,\phi,\psi,t} \delta.
\end{aligned} \tag{436}$$

Since $\delta > 0$ was arbitrary we conclude from (435)

$$\lim_{x \to +\infty} \langle k^{\epsilon}_{P_t^+}(x,x)\,\phi,\psi\rangle_H = (4\pi\,(t+2\epsilon))^{-1/2}\,\langle e^{-\epsilon A_-^2} A_+ e^{-tA_+^2} e^{-\epsilon A_-^2}\phi,\psi\rangle_H, \tag{437}$$

and from (436)

$$\lim_{x \to +\infty} \langle k^{\epsilon}_{Q_t^+}(x,x)\,\phi,\psi\rangle_H = t^{-1}\int_0^t (4\pi\,(s+2\epsilon))^{-1/2}\,\langle e^{-\epsilon A_-^2} A_+ e^{-sA_+^2} e^{-\epsilon A_-^2}\phi,\psi\rangle_H \mathrm{d}s, \tag{438}$$

Formula (425) yields

$$\int_0^t (4\pi\,(s+2\epsilon))^{-1/2}\, z e^{-sz^2}\mathrm{d}s = \chi_{t,2\epsilon}(z)\,. \tag{439}$$

Therefore (438) can be restated as

$$\lim_{x \to +\infty} \langle k^{\epsilon}_{Q_t^+}(x,x)\,\phi,\psi\rangle_H = t^{-1}\langle e^{-\epsilon A_-^2}\chi_{t,2\epsilon}(A_+)\,e^{-\epsilon A_-^2}\phi,\psi\rangle_H. \tag{440}$$

■

We are now able to harvest the first trace formula by virtue of the previous Theorem 4.10 and Proposition 4.11.

Proposition 4.12. *Assume Hypothesis A2 (*2.11*) and either Hypothesis B1 (*2.12*) or Hypothesis B2 (*2.14*). Let $\epsilon, t > 0$ then*

$$\begin{aligned}
A_+ e^{-tA_+^2} - A_- e^{-tA_-^2} &\in S^1(H)\,,\\
\mathrm{tr}_{L^2(\mathbb{R},H)}\left(\{[\partial, P_t^+]\}\right) &= (4\pi t)^{-1/2}\,\mathrm{tr}_H\left(A_+ e^{-tA_+^2} - A_- e^{-tA_-^2}\right),\\
k^{\epsilon}_{P_t^+}(x,x) - (4\pi t)^{-1/2} A_- e^{-(t+2\epsilon)A_-^2} &\in S^1(H)\,, \quad \textit{for all } x \in \mathbb{R},\\
\left\| k^{\epsilon}_{P_t^+}(x,x) - (4\pi t)^{-1/2} A_- e^{-(t+2\epsilon)A_-^2}\right\|_{S^1(H)} &\le \left\|\{[\partial, P_t^+]\}\right\|_{S^1(L^2(\mathbb{R},H))}, \quad \textit{for all } x \in \mathbb{R}.
\end{aligned} \tag{441}$$

Proof. Hypothesis A2 (2.11) implies that for

$$g(s,t) := \int_{\mathbb{R}} \left\| e^{-sA_-^2} A'(x)\, e^{-tA_-^2}\right\|_{S^1(H)} \mathrm{d}x, \tag{442}$$

we have $g \in I_{-1/2,0}$ and thus, by the trace formula 200 of Proposition 3.6, that

$$f(A_+) - f(A_-) \in S^1(H)\,, \tag{443}$$

where f is twice weakly differentiable with locally bounded derivatives and there is $r > 1$ such that

$$\left(\nu^2 f'(\nu)\right)' =_{|\nu|\to\infty} O\left(|\nu|^{-1-r}\right),$$

$$\lim_{\nu\to-\infty} f(\nu) = \lim_{\nu\to+\infty} f(\nu), \quad \lim_{\nu\to\pm\infty} \nu^2 f'(\nu) = 0. \tag{444}$$

We easily verify that $f(\nu) := \nu e^{-t\nu^2}$ satisfies condition (444) and thus, by (443) we conclude

$$A_+ e^{-tA_+^2} - A_- e^{-tA_-^2} \in S^1(H), \tag{445}$$

which is the first statement of (441).
Since $\{[\partial, P_t^+]\}$ is trace-class in $L^2(\mathbb{R}, H)$, by Theorem 3.21, statement (393) of Theorem 4.10 implies that

$$\lim_{(y,y_0)\to(x,x_0)} k^\epsilon_{P_t^+}(x,x) - k^\epsilon_{P_t^+}(x_0,x_0) \in S^1(H), \text{ for } x, x_0 \in \mathbb{R}\cup\{\pm\infty\}, \tag{446}$$

which must coincide, for $x = +\infty$ and $x_0 = -\infty$, with the weak limits derived in Proposition 4.11 and therefore, by statement (394) of Theorem 4.10, we have

$$\operatorname{tr}_{L^2(\mathbb{R},H)}\left(\{[\partial, P_t^+]\}\right) = (4\pi t)^{-1/2} \lim_{\epsilon\searrow 0} \operatorname{tr}_H\left(e^{-\epsilon A_-^2}\left(A_+ e^{-tA_+^2} - A_- e^{-tA_-^2}\right) e^{-\epsilon A_-^2}\right). \tag{447}$$

On the other hand, we have (445). Since $e^{-\epsilon A_-^2}$ is self-adjoint and converges strongly to 1 in H, we conclude by Lemma 4.3 that we may interchange trace and limit in (447) and thus

$$\operatorname{tr}_{L^2(\mathbb{R},H)}\left(\{[\partial, P_t^+]\}\right) = (4\pi t)^{-1/2} \operatorname{tr}_H\left(A_+ e^{-tA_+^2} - A_- e^{-tA_-^2}\right), \tag{448}$$

which is the second statement of (441).
Proposition 4.11 and (446) also immediately imply that

$$k^\epsilon_{P_t^+}(x,x) - (4\pi t)^{-1/2} A_- e^{-(t+2\epsilon)A_-^2} \in S^1(H), \quad \text{for all } x \in \mathbb{R}, \tag{449}$$

giving us the third statement of (441).
Theorem 4.10 and Proposition 4.11 finally implies the last statement of (441),

$$\left\| k^\epsilon_{P_t^+}(x,x) - (4\pi t)^{-1/2} A_- e^{-(t+2\epsilon)A_-^2} \right\|_{S^1(H)} \le \left\| \{[\partial, P_t^+]\} \right\|_{S^1(L^2(\mathbb{R},H))}, \quad \text{for all } x \in \mathbb{R}. \tag{450}$$

■

Similarly we obtain a trace formula concerned with the commutator of ∂ and Q_t^+ using Proposition 4.11 and Theorem 4.10.

Proposition 4.13. *Assume Hypothesis A2 (*2.11*) and either Hypothesis B1 (*2.12*) or Hypothesis B2 (*2.14*). Let $\epsilon, t > 0$ then*

$$\operatorname{tr}_{L^2(\mathbb{R},H)}\left(e^{-\epsilon H_0}\left[\partial, Q_t^+\right] e^{-\epsilon H_0}\right) = t^{-1} \operatorname{tr}_H\left(e^{-\epsilon A_-^2}\left(\chi_{t,2\epsilon}(A_+) - \chi_{t,2\epsilon}(A_-)\right) e^{-\epsilon A_-^2}\right),$$
$$k^\epsilon_{Q_t^+}(x,x) - t^{-1} e^{-\epsilon A_-^2} \chi_{t,2\epsilon}(A_-) e^{-\epsilon A_-^2} \in S^1(H) \text{ for } x \in \mathbb{R}\cup\{\pm\infty\}. \tag{451}$$

Proof. The operator $e^{-\epsilon H_0}\left\{\left[\partial, Q_t^+\right]\right\}e^{-\epsilon H_0}$ is trace-class in $L^2(\mathbb{R}, H)$, by Theorem 3.22. Analogous to the proof of Theorem 4.10 one concludes that

$$\lim_{(y,y_0)\to(x,x_0)} k^\epsilon_{Q_t^+}(x,x) - k^\epsilon_{Q_t^+}(x_0,x_0) \in S^1(H),\ \text{for } x, x_0 \in \mathbb{R}\cup\{\pm\infty\}, \tag{452}$$

and

$$\operatorname{tr}_{L^2(\mathbb{R},H)}\left(e^{-\epsilon H_0}\left[\partial, Q_t^+\right]e^{-\epsilon H_0}\right) = \operatorname{tr}_H\left(\lim_{(x_1,x_0)\to(+\infty,-\infty)} k^\epsilon_{Q_t^+}(x_1,x_1) - k^\epsilon_{Q_t^+}(x_0,x_0)\right). \tag{453}$$

The limits in (452) must coincide with the weak limits derived in Proposition 4.11 and therefore we have

$$k^\epsilon_{Q_t^+}(x,x) - t^{-1}e^{-\epsilon A_-^2}\chi_{t,2\epsilon}(A_-)\,e^{-\epsilon A_-^2} \in S^1(H)\ \text{ for } x\in\mathbb{R}\cup\{\pm\infty\}, \tag{454}$$

and

$$\operatorname{tr}_{L^2(\mathbb{R},H)}\left(e^{-\epsilon H_0}\left[\partial, Q_t^+\right]e^{-\epsilon H_0}\right) = t^{-1}\operatorname{tr}_H\left(e^{-\epsilon A_-^2}\left(\chi_{t,2\epsilon}(A_+) - \chi_{t,2\epsilon}(A_-)\right)e^{-\epsilon A_-^2}\right). \tag{455}$$

■

After consideration of the commutator with ∂, it remains for us to discuss the commutators of P_t^+ and Q_t^+ with $A(X)$ to obtain the trace formulae (1), reminding us of the decompositions in Lemma 2.32 and Theorem 3.22. We start by showing that a commutator with $A(X)$ can only contribute purely imaginary in trace.

Lemma 4.14. *Let $T \in B\left(L^2(\mathbb{R},H), \operatorname{Dom}\left(\widehat{A_-}\right)_\Gamma\right)$ be a self-adjoint operator in $L^2(\mathbb{R},H)$ and assume that $\{TA(X)\}$ exists, then for $\epsilon > 0$ and $\phi \in H$ we have for $x \in \mathbb{R}$*

$$\langle k^\epsilon_{\{[A(X),T]\}}(x,x)\,\phi,\phi\rangle_H \in i\cdot\mathbb{R}. \tag{456}$$

Proof. Denote $f_\epsilon^{\phi,x} := q_\epsilon(x-\cdot)\otimes e^{-\epsilon A_-^2}\phi$. We remark that $f_\epsilon^{\phi,x} \in \operatorname{Dom}\left(\widehat{A_-}\right)$. Since $\{[A(X),T]\}$ is a bounded operator in $L^2(\mathbb{R},H)$, we have by Proposition 4.5,

$$\begin{aligned}
&\langle k^\epsilon_{\{[A(X),T]\}}(x,x)\,\phi,\phi\rangle_H\\
=&\int_{\mathbb{R}}\int_{\mathbb{R}} q_\epsilon(x-z_1)\,q_\epsilon(x-z_2)\,\langle e^{-\epsilon A_-^2}\theta^{\{[A(X),T]\}}_{e^{-\epsilon A_-^2}\phi}(z_1,z_2),\phi\rangle_H \mathrm{d}z_2\,\mathrm{d}z_1\\
=&\langle\theta^{\{[A(X),T]\}}_{e^{-\epsilon A_-^2}\phi}, q_\epsilon(x-\cdot)\otimes\left(e^{-\epsilon A_-^2}\phi\right)\otimes q_\epsilon(x-\cdot)\rangle_{L^2(\mathbb{R}^2,H)}\\
=&\langle[A(X),T]\,f_\epsilon^{\phi,x}, f_\epsilon^{\phi,x}\rangle_{L^2(\mathbb{R},H)}\\
=&\langle Tf_\epsilon^{\phi,x}, A(X)\,f_\epsilon^{\phi,x}\rangle_{L^2(\mathbb{R},H)} - \langle A(X)\,f_\epsilon^{\phi,x}, Tf_\epsilon^{\phi,x}\rangle_{L^2(\mathbb{R},H)}\\
=&2i\Im\left(\langle Tf_\epsilon^{\phi,x}, A(X)\,f_\epsilon^{\phi,x}\rangle_{L^2(\mathbb{R},H)}\right)\in i\cdot\mathbb{R}.
\end{aligned}\tag{457}$$

■

We immediately conclude, keeping the decompositions in Lemma 2.32 and Theorem 3.22 in mind, that the trace of the commutators of P_t^+ and Q_t^+ with $A(X)$ need to vanish.

Corollary 4.15. *Assume Hypothesis A2 (*2.11*) and either Hypothesis B1 (*2.12*) or Hypothesis B2 (*2.14*) and let $\epsilon, t > 0$. Then*

$$\begin{aligned} \operatorname{tr}_{L^2(\mathbb{R},H)}\left(e^{-\epsilon H_0}\left[A(X), P_t^+\right]e^{-\epsilon H_0}\right) &= 0, \\ \operatorname{tr}_{L^2(\mathbb{R},H)}\left(e^{-\epsilon H_0}\left[A(X), Q_t^+\right]e^{-\epsilon H_0}\right) &= 0. \end{aligned} \tag{458}$$

Proof. By Theorem 3.22, respectively Theorem 3.21, we know that the operators $e^{-\epsilon H_0}\left[A(X), Q_t^+\right]e^{-\epsilon H_0}$ and $e^{-\epsilon H_0}\left[A(X), P_t^+\right]e^{-\epsilon H_0}$ are trace-class in $L^2(\mathbb{R}, H)$. By the Trace Lemma 4.1 and Proposition 4.8 we thus infer for $T = P_t^+$ or $T = Q_t^+$, and an orthonormal basis $(e_n)_{n\in\mathbb{N}}$ of H, that

$$\begin{aligned} \operatorname{tr}_{L^2(\mathbb{R},H)}\left(e^{-\epsilon H_0}\left[A(X), T\right]e^{-\epsilon H_0}\right) &= \int_{\mathbb{R}} \operatorname{tr}_H\left(k^{\epsilon}_{\{[A(X),T]\}}(x,x)\right)\mathrm{d}x \\ &= \int_{\mathbb{R}} \sum_{n\in\mathbb{N}} \langle k^{\epsilon}_{\{[A(X),T]\}}(x,x)\, e_n, e_n\rangle_H \mathrm{d}x \\ &\in i\cdot\mathbb{R}, \end{aligned} \tag{459}$$

where in the last step we used Lemma 4.14 (it is easily checked that P_t^+ and Q_t^+ indeed satisfy the prerequisites).
On the other hand we know by Theorem 3.22 and Proposition 4.13 that

$$\begin{aligned} & - t\cdot\operatorname{tr}_{L^2(\mathbb{R},H)}\left(e^{-\epsilon H_0}\left[A(X), Q_t^+\right]e^{-\epsilon H_0}\right) \\ =& \operatorname{tr}_{L^2(\mathbb{R},H)}\left(e^{-\epsilon H_0}\left(e^{-tH_+} - e^{-tH_-}\right)e^{-\epsilon H_0}\right) + t\cdot\operatorname{tr}_{L^2(\mathbb{R},H)}\left(e^{-\epsilon H_0}\left[\partial, Q_t^+\right]e^{-\epsilon H_0}\right) \\ =& \operatorname{tr}_{L^2(\mathbb{R},H)}\left(e^{-\epsilon H_0}\left(e^{-tH_+} - e^{-tH_-}\right)e^{-\epsilon H_0}\right) + \operatorname{tr}_H\left(e^{-\epsilon A_-^2}\left(\chi_{t,2\epsilon}(A_+) - \chi_{t,2\epsilon}(A_-)\right)e^{-\epsilon A_-^2}\right) \\ \in& \mathbb{R}, \end{aligned} \tag{460}$$

where in the last step of (460) we used the observation that the operators in the traces in the penultimate line of (460) are self-adjoint in $L^2(\mathbb{R}, H)$ respectively in H, therefore the traces take real values.
Similarly one shows that

$$\operatorname{tr}_{L^2(\mathbb{R},H)}\left(e^{-\epsilon H_0}\left[A(X), P_t^+\right]e^{-\epsilon H_0}\right) \in \mathbb{R}. \tag{461}$$

Combining (460) and (461) with (459), we conclude that the traces must be 0, proving (458). ∎

To conclude the chapter, we are now finally able to state and proof the trace formulae (1) with the correct assumptions.

Theorem 4.16. *Assume Hypothesis A2 (*2.11*) and either Hypothesis B1 (*2.12*) or Hypothesis B2 (*2.14*) and let $t > 0$. Then*

$$\operatorname{tr}_{S^1(L^2(\mathbb{R},H))}\left(H_+e^{-tH_+} - H_-e^{-tH_-}\right) = (4\pi t)^{-1/2}\operatorname{tr}_{S^1(H)}\left(A_+e^{-tA_+^2} - A_-e^{-tA_-^2}\right). \tag{462}$$

Proof. We conclude using Lemma 4.3, Proposition 4.12, and Corollary 4.15,

$$\begin{aligned}
&\operatorname{tr}_{S^1(L^2(\mathbb{R},H))}\left(H_+e^{-tH_+}-H_-e^{-tH_-}\right)\\
=&\lim_{\epsilon\searrow 0}\operatorname{tr}_{S^1(L^2(\mathbb{R},H))}\left(e^{-\epsilon H_0}\left(H_+e^{-tH_+}-H_-e^{-tH_-}\right)e^{-\epsilon H_0}\right)\\
=&\lim_{\epsilon\searrow 0}\operatorname{tr}_{S^1(L^2(\mathbb{R},H))}\left(e^{-\epsilon H_0}\left[\partial,P_t^+\right]e^{-\epsilon H_0}\right)+\lim_{\epsilon\searrow 0}\operatorname{tr}_{S^1(L^2(\mathbb{R},H))}\left(e^{-\epsilon H_0}\left[A\left(X\right),P_t^+\right]e^{-\epsilon H_0}\right)\\
=&\operatorname{tr}_{S^1(L^2(\mathbb{R},H))}\left(\left\{\left[\partial,P_t^+\right]\right\}\right)+0\\
=&\left(4\pi t\right)^{-1/2}\operatorname{tr}_H\left(A_+e^{-tA_+^2}-A_-e^{-tA_-^2}\right).
\end{aligned}\tag{463}$$

■

Theorem 4.17. *Assume Hypothesis A2 (*2.11*) and either Hypothesis B1 (*2.12*) or Hypothesis B2 (*2.14*) and let* $t>0$*. Then*

$$\operatorname{tr}_{S^1(L^2(\mathbb{R},H))}\left(e^{-tH_+}-e^{-tH_-}\right)=-\lim_{\epsilon\searrow 0}\operatorname{tr}_H\left(e^{-\epsilon A_-^2}\left(\chi_{t,2\epsilon}\left(A_+\right)-\chi_{t,2\epsilon}\left(A_-\right)\right)e^{-\epsilon A_-^2}\right).$$

Proof. We conclude using Lemma 4.3, Theorem 3.22, Proposition 4.13 and Corollary 4.15

$$\begin{aligned}
&\operatorname{tr}_{S^1(L^2(\mathbb{R},H))}\left(e^{-tH_+}-e^{-tH_-}\right)=\lim_{\epsilon\searrow 0}\operatorname{tr}_{S^1(L^2(\mathbb{R},H))}\left(e^{-\epsilon H_0}\left(e^{-tH_+}-e^{-tH_-}\right)e^{-\epsilon H_0}\right)\\
=&-t\lim_{\epsilon\searrow 0}\operatorname{tr}_{S^1(L^2(\mathbb{R},H))}\left(e^{-\epsilon H_0}\left[\partial,Q_t^+\right]e^{-\epsilon H_0}\right)\\
&-t\lim_{\epsilon\searrow 0}\operatorname{tr}_{S^1(L^2(\mathbb{R},H))}\left(e^{-\epsilon H_0}\left[A\left(X\right),Q_t^+\right]e^{-\epsilon H_0}\right)\\
=&-t\lim_{\epsilon\searrow 0}\operatorname{tr}_{S^1(L^2(\mathbb{R},H))}\left(e^{-\epsilon H_0}\left[\partial,Q_t^+\right]e^{-\epsilon H_0}\right)-0\\
=&-\lim_{\epsilon\searrow 0}\operatorname{tr}_H\left(e^{-\epsilon A_-^2}\left(\chi_{t,2\epsilon}\left(A_+\right)-\chi_{t,2\epsilon}\left(A_-\right)\right)e^{-\epsilon A_-^2}\right).
\end{aligned}\tag{464}$$

■

5 A Pushnitski-type formula and the Witten index of D

In the last chapter, we proved Theorem 4.16 and Theorem 4.17, which gave us the trace formulae (1). These equations, connecting the $L^2(\mathbb{R}, H)$-traces of differences of functions of $H_\pm$ with H-traces of differences of functions of $A_\pm$, generate a functional relation between the spectral shift functions constructed in chapter 3. This functional equation is necessarily a version of Pushnitski's formula, up to a normalization constant.
If we fix the normalization of the spectral shift function of the pair (A_+, A_-) under the spectral gap assumption $0 \in \rho(A_-) \cap \rho(A_+)$, we determine this normalization constant and it turns out to be the Witten index of D under this additional statement (in general the Witten index might not exist). Let us therefore first define the (semi-group regularized) Witten index abstractly, according to [17].

Definition 5.1. Let T be a densely defined, closed operator in a complex, separable Hilbert space X. Then the self-adjoint operators T^*T and TT^* are non-negative in X, and, if the limit

$$\operatorname{ind}_W(T) := \lim_{t\to+\infty} \operatorname{tr}_X \left(e^{-tT^*T} - e^{-tTT^*}\right), \tag{465}$$

exists, we say that T possesses the (semi-group regularized) Witten index $\operatorname{ind}_W(T)$.

Remark 5.2. It should be noted that if T is additionally Fredholm in X, the Witten index of T exists and coincides with the Fredholm index of T (c.f. [17]), which shows that the Witten index is a generalization of the Fredholm index.
Although more general than the Fredholm index, the Witten index still retains some invariance properties under perturbation (c.f. [17, Corollary 3.2]).

Theorem 5.3. *Assume Hypothesis A2 (*2.11*) and either Hypothesis B1 (*2.12*) or Hypothesis B2 (*2.14*). Then there exists a constant $\kappa \in \mathbb{R}$, such that for a.e. $\lambda > 0$*

$$\xi(\lambda, H_+, H_-) = \kappa + \frac{1}{\pi}\int_{-\lambda^{1/2}}^{+\lambda^{1/2}} \xi(\mu, A_+, A_-)\left(\lambda - \mu^2\right)^{-1/2} \mathrm{d}\mu, \tag{466}$$

where the spectral shift functions $\xi(\cdot, H_+, H_-)$ and $\xi(\cdot, A_+, a_-)$ are defined according to Definition 3.23 *and Proposition* 3.6 *respectively.*

If additionally $0 \in \rho(A_+) \cap \rho(A_-)$, then the semi-group regularized Witten index of D, $\operatorname{ind}_W(D)$, exists and we have

$$\xi(\lambda, H_+, H_-) = \operatorname{ind}_W(D) + \frac{1}{\pi}\int_{-\lambda^{1/2}}^{+\lambda^{1/2}} \eta(\mu, A_+, A_-)\left(\lambda - \mu^2\right)^{-1/2} \mathrm{d}\mu, \tag{467}$$

where $\eta(\cdot, A_+, A_-)$ is defined according to Definition 3.8*. Then a.e. in a non-negative neighbourhood of* 0 *we have*

$$\xi(\cdot, H_+, H_-) \equiv \operatorname{ind}_W(D). \tag{468}$$

We then also obtain the index formula

$$\operatorname{ind}_W(D) = \lim_{t\to+\infty}\lim_{\epsilon\searrow 0} \operatorname{tr}_H\left(e^{-\epsilon A_-^2}\left(\chi_{t,2\epsilon}(A_+) - \chi_{t,2\epsilon}(A_-)\right)e^{-\epsilon A_-^2}\right). \tag{469}$$

Proof. For this proof denote $\xi_{H_\pm} = \xi(\cdot, H_+, H_-)$, $\xi_{A_\pm} = \xi(\cdot, A_+, A_-)$ and $\eta = \eta(\cdot, A_+, A_-)$. By Remark 3.29 we note that the functions $f_t(\lambda) := \lambda e^{-t\lambda}$ are amenable for the spectral shift function trace formula of the pair (H_+, H_-) for $t > 0$, i.e.

$$\operatorname{tr}_{L^2(\mathbb{R},H)}\left(H_+e^{-tH_+} - H_-e^{-tH_-}\right) = \int_0^\infty (1 - t\lambda)\, e^{-t\lambda}\xi(\lambda)\,\mathrm{d}\lambda. \tag{470}$$

We note also that the functions $g_t(\mu) := (4\pi t)^{-1/2}\mu\ e^{-t\mu^2}$, $t > 0$, are amenable for the trace formulae (203) and (215) of the spectral shift function of the pair (A_+, A_-) defined in Proposition 3.6 and in Definition 3.8, respectively, for $t > 0$, i.e.

$$\begin{aligned}(4\pi t)^{-1/2}\operatorname{tr}_H\left(A_+e^{-tA_+^2} - A_-e^{-tA_-^2}\right) &= \int_{\mathbb{R}} (4\pi t)^{-1/2}\left(1 - 2t\mu^2\right)e^{-t\mu^2}\eta(\mu)\,\mathrm{d}\mu \\ &= \int_{\mathbb{R}} (4\pi t)^{-1/2}\left(1 - 2t\mu^2\right)e^{-t\mu^2}\xi_{A_\pm}(\mu)\,\mathrm{d}\mu. \end{aligned}\tag{471}$$

By Theorem 4.16, we therefore have for $t > 0$ that

$$\begin{aligned}\int_0^\infty (1 - t\lambda)\, e^{-t\lambda}\xi_{H_\pm}(\lambda)\,\mathrm{d}\lambda &= \int_{\mathbb{R}} (4\pi t)^{-1/2}\left(1 - 2t\mu^2\right)e^{-t\mu^2}\eta(\mu)\,\mathrm{d}\mu \\ &= \int_{\mathbb{R}} (4\pi t)^{-1/2}\left(1 - 2t\mu^2\right)e^{-t\mu^2}\xi_{A_\pm}(\mu)\,\mathrm{d}\mu. \end{aligned}\tag{472}$$

By the L^1-memberships of $\xi_{H_\pm}$ (cf. Remark 3.29), of η (cf. Proposition 3.6), and of $\xi_{A_\pm}$ (cf. Proposition 3.9), we see that we may integrate both sides of (472) in t from t_0 to t_1, where $0 < t_0 < t_1 < \infty$, and we may interchange the order of integration by Fubini's theorem. We obtain therefore

$$\begin{aligned}\int_0^\infty \left(t_1e^{-t_1\lambda} - t_0e^{-t_0\lambda}\right)\xi_{H_\pm}(\lambda)\,\mathrm{d}\lambda &= \int_{\mathbb{R}}\left(\left(\frac{t_1}{\pi}\right)^{1/2}e^{-t_1\mu^2} - \left(\frac{t_0}{\pi}\right)^{1/2}e^{-t_0\mu^2}\right)\eta(\mu)\,\mathrm{d}\mu \\ &= \int_{\mathbb{R}}\left(\left(\frac{t_1}{\pi}\right)^{1/2}e^{-t_1\mu^2} - \left(\frac{t_0}{\pi}\right)^{1/2}e^{-t_0\mu^2}\right)\xi_{A_\pm}(\mu)\,\mathrm{d}\mu. \end{aligned}\tag{473}$$

Since $(\pi/t)^{1/2} = \int_0^\infty e^{-st}s^{-1/2}\mathrm{d}s$, we have (keeping in mind the integrability properties of η and $\xi_{A_\pm}$,) for $t > 0$,

$$\begin{aligned}\int_{\mathbb{R}}\left(\frac{t}{\pi}\right)^{1/2}e^{-t\mu^2}\eta(\mu)\,\mathrm{d}\mu &= \frac{t}{\pi}\int_{\mathbb{R}} e^{-t\mu^2}\int_0^\infty e^{-st}s^{-1/2}\mathrm{d}s\ \eta(\mu)\,\mathrm{d}\mu \\ &= \frac{t}{\pi}\int_{\mathbb{R}}\int_0^\infty \mathbb{1}_{\{s>\mu^2\}}e^{-st}\left(s - \mu^2\right)^{-1/2}\mathrm{d}s\ \eta(\mu)\,\mathrm{d}\mu \\ &= t\int_0^\infty e^{-st}\left(\frac{1}{\pi}\int_{-s^{1/2}}^{s^{1/2}}\frac{\eta(\mu)}{(s - \mu^2)^{1/2}}\mathrm{d}\mu\right)\mathrm{d}s, \end{aligned}$$

$$\int_{\mathbb{R}}\left(\frac{t}{\pi}\right)^{1/2}e^{-t\mu^2}\xi_{A_\pm}(\mu)\,\mathrm{d}\mu = \frac{t}{\pi}\int_{\mathbb{R}} e^{-t\mu^2}\int_0^\infty e^{-st}s^{-1/2}\mathrm{d}s\ \eta(\mu)\,\mathrm{d}\mu$$

$$= \frac{t}{\pi}\int_{\mathbb{R}}\int_0^\infty \mathbb{1}_{\{s>\mu^2\}} e^{-st}\left(s-\mu^2\right)^{-1/2} \mathrm{d}s\, \xi_{A_\pm}(\mu)\,\mathrm{d}\mu$$
$$= t\int_0^\infty e^{-st}\left(\frac{1}{\pi}\int_{-s^{1/2}}^{s^{1/2}} \frac{\xi_{A_\pm}(\mu)}{\left(s-\mu^2\right)^{1/2}}\mathrm{d}\mu\right)\mathrm{d}s. \tag{474}$$

We define

$$\zeta_\eta(s) := \frac{1}{\pi}\int_{-s^{1/2}}^{s^{1/2}} \frac{\eta(\mu)}{\left(s-\mu^2\right)^{1/2}}\mathrm{d}\mu,\ \zeta_\xi(s) := \frac{1}{\pi}\int_{-s^{1/2}}^{s^{1/2}} \frac{\xi_{A_\pm}(\mu)}{\left(s-\mu^2\right)^{1/2}}\mathrm{d}\mu. \tag{475}$$

By putting (474) into (473) we conclude that for $t_1 > 0$ we have

$$\int_0^\infty e^{-t_1\lambda}\xi_{H_\pm}(\lambda)\,\mathrm{d}\lambda = \int_0^\infty e^{-t_1 s}\zeta_\eta(s)\,\mathrm{d}s + \frac{\kappa_{t_0}^\eta}{t_1} = \int_0^\infty e^{-t_1 s}\zeta_\xi(s)\,\mathrm{d}s + \frac{\kappa_{t_0}^\xi}{t_1}, \tag{476}$$

or put differently

$$\int_0^\infty e^{-t_1\lambda}\left(\xi_{H_\pm}(\lambda) - \zeta_\eta(\lambda) - \kappa_{t_0}^\eta\right)\mathrm{d}\lambda = \int_0^\infty e^{-t_1\lambda}\left(\xi_{H_\pm}(\lambda) - \zeta_\xi(\lambda) - \kappa_{t_0}^\xi\right)\mathrm{d}\lambda = 0, \tag{477}$$

where

$$\kappa_{t_0}^\eta := t_0\int_0^\infty e^{-t_0 s}\left(\xi_{H_\pm}(s) - \zeta_\eta(s)\right)\mathrm{d}s,$$
$$\kappa_{t_0}^\xi := t_0\int_0^\infty e^{-t_0 s}\left(\xi_{H_\pm}(s) - \zeta_\xi(s)\right)\mathrm{d}s, \tag{478}$$

Thus by Lerch's theorem (cf. [25]) on the uniqueness of the Laplace transform inversion we conclude that there are constants $\kappa^\eta := \kappa_{t_0}^\eta$, $\kappa^\xi := \kappa_{t_0}^\xi$ (independent of t_0 though), such that

$$\xi_{H_\pm} = \zeta_\eta + \kappa^\eta = \zeta_\xi + \kappa^\xi, \quad \text{a.e.}. \tag{479}$$

If we additionally assume that $0 \in \rho(A_-) \cap \rho(A_+)$, then η is constantly 0 on a neighbourhood of 0 (say on $(-\epsilon, \epsilon)$ for some $\epsilon > 0$) by Proposition 3.9. Revisiting the right hand side of equation (473), we obtain in this case

$$\left|\int_{\mathbb{R}}\left(\frac{t_1}{\pi}\right)^{1/2} e^{-t_1\mu^2}\eta(\mu)\,\mathrm{d}\mu\right| = \left|\int_{\mathbb{R}\setminus(-\epsilon,\epsilon)}\left(\frac{t_1}{\pi}\right)^{1/2} e^{-t_1\mu^2}\left(\mu^2+1\right)\left(\mu^2+1\right)^{-1}\eta(\mu)\,\mathrm{d}\mu\right|$$
$$\leq \|\eta\|_{L^1\left(\mathbb{R},(\mu^2+1)^{-1}\mathrm{d}\mu\right)} \cdot \sup_{|x|\geq\epsilon}\left(\frac{t_1}{\pi}\right)^{1/2} e^{-t_1x^2}\left(x^2+1\right). \tag{480}$$

If $t_1 > 1$, there exist no extreme point of the function $x \mapsto e^{-t_1x^2}\left(x^2+1\right)$ on $\mathbb{R}\setminus(-\epsilon,\epsilon)$. Since $\lim_{x\to\infty} e^{-t_1x^2}\left(x^2+1\right) = 0$, we conclude that

$$\left|\int_{\mathbb{R}}\left(\frac{t_1}{\pi}\right)^{1/2} e^{-t_1\mu^2}\eta(\mu)\,\mathrm{d}\mu\right| \leq \|\eta\|_{L^1\left(\mathbb{R},(\mu^2+1)^{-1}\mathrm{d}\mu\right)} \cdot \left(\frac{t_1}{\pi}\right)^{1/2} e^{-t_1\epsilon^{-2}}\left(\epsilon^{-2}+1\right)$$
$$\xrightarrow{t_1\to\infty} 0. \tag{481}$$

This means that also the limit for $t_1 \to +\infty$ on the left hand side of equation (473) must exist. This implies that

$$\lim_{t_1 \to +\infty} \int_0^\infty t_1 e^{-t_1 \lambda} \xi_{H_\pm}(\lambda)\,\mathrm{d}\lambda$$

exists. By virtue of the trace formula in Lemma 3.27 and Remark 3.29 we conclude that the limit

$$\begin{aligned}\lim_{t_1 \to \infty} \int_0^\infty t_1 e^{-t_1 \lambda} \xi_{H_\pm}(\lambda)\,\mathrm{d}\lambda &= \lim_{t_1 \to \infty} \mathrm{tr}_{L^2(\mathbb{R},H)} \left(e^{-tH_-} - e^{-tH_+}\right) \\ &= \lim_{t_1 \to +\infty} \int_0^\infty t_1 e^{-t_1 \lambda} \xi_{H_\pm}(\lambda)\,\mathrm{d}\lambda. \end{aligned} \tag{482}$$

also exists. Since $H_- = D^* D$ and $H_+ = DD^*$, we conclude that the semi-group regularized Witten index, of D, $\mathrm{ind}_W(D)$, exists and by Theorem 4.17 we conclude

$$\mathrm{ind}_W(D) = \lim_{t \to +\infty} \lim_{\epsilon \searrow 0} \mathrm{tr}_H \left(e^{-\epsilon A_-^2} \left(\chi_{t,2\epsilon}(A_+) - \chi_{t,2\epsilon}(A_-)\right) e^{-\epsilon A_-^2}\right). \tag{483}$$

Furthermore we find

$$\kappa^\eta \equiv \kappa^\eta_{t_0} = \lim_{t_0 \to \infty} t_0 \int_0^\infty e^{-t_0 s} \left(\xi_{H_\pm}(s) - \zeta_\eta(s)\right) \mathrm{d}s = \mathrm{ind}_W(D), \tag{484}$$

where we substituted back equation 474 and used 481. Finally, since ζ_η is constant 0 in neighbourhood of 0 (since η is), we conclude that $\xi_{H_\pm} = \mathrm{ind}_W(D)$ a.e. in a non-negative neighbourhood of 0. ■

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