ON THE RELATIONSHIP OF SPECTRAL FLOW TO THE FREDHOLM INDEX AND ITS EXTENSION TO NON-FREDHOLM OPERATORS

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Abstract. In [APS76] Atiyah, Patodi and Singer introduced spectral flow for elliptic operators on odd dimensional compact manifolds. They argued that it could be computed from the Fredholm index of an elliptic operator on a manifold of one higher dimension. A general proof of this fact was produced by Robbin-Salamon [RS95]. In [GLM+11], a start was made on extending these ideas to operators with some essential spectrum as occurs on non-compact manifolds. The new ingredient introduced there was to exploit scattering theory following the fundamental paper [Pus08]. These results do not apply to differential operators directly, only to pseudo-differential operators on manifolds, due to the restrictive assumption that spectral flow is considered between an operator and its perturbation by a relatively trace-class operator. In this paper we extend the main results of these earlier papers to spectral flow between an operator and a perturbation satisfying a higher $p^{th}$ Schatten class condition for $0 \leq p < \infty$, thus allowing differential operators on manifolds of any dimension $d < p + 1$. In fact our main result does not assume any ellipticity or Fredholm properties at all and proves an operator theoretic trace formula motivated by [BCP+06, CGK16]. This leads us to introduce a notion of ‘generalised spectral flow’ for such paths and to investigate its properties.

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1. Introduction

1.1. Motivation and background. The notion of spectral flow for paths of self-adjoint elliptic operators was introduced in Atiyah–Patodi–Singer [APS76]. There they explained how one might compute it by using a 'suspension' trick that produces a first order elliptic operator on a manifold of one higher dimension whose Fredholm index was equal to the spectral flow along the original path. Analogous theorems were later studied by other methods (see for example [BBW93]) culminating in a definitive treatment for certain self-adjoint differential operators with compact resolvent in a paper of Robbin–Salamon, [RS95]. Their paper has implications for many applications including those to Morse theory, Floer homology, Morse and Maslov indices, Cauchy-Riemann operators, and all the way to oscillation theory.

Spectral flow in the early works [APS76], [RS95] is treated in a topological fashion and in particular, K-theoretically in [RS95]. A new, purely analytic approach to spectral flow was introduced in [Phi96]. Combined with the viewpoint of [Get93] this produced analytic formulas for spectral flow [CP98, CP04], providing an analytic counterpoint to the previous K-theoretic and intersection number approaches. This opened the way to an analytic formulation of the Robbin-Salamon theorem. A first step in this direction was the introduction in [BCP+06] of an operator theoretic trace formula that gives a version of the Robbin-Salamon result proved in the setting of Atiyah’s $L^2$ index theorem (that is it uses the notion ‘von Neumann spectral flow’ that arises in semi-finite von Neumann algebras). All of these results however assume that the unbounded Fredholm operators whose spectral flow is computed have compact resolvents (in the sense of semifinite von Neumann algebras).

With the exception of [BCP+06], the focus in mathematics on these questions has been mainly on geometrically defined operators associated to compact manifolds. Physicists, however, are interested in the case of non-compact manifolds and non-geometric examples. The stumbling block for index formulas in that situation is the presence of essential spectrum. Motivated by ideas from scattering theory an approach to a Robbin-Salamon type result for paths of self-adjoint Fredholm operators with some essential spectrum was initiated in [Pus08], followed by [GLM+11]. However, the key assumption in [GLM+11] is that spectral flow is only considered between self-adjoint operators that differ by a so-called relatively trace class perturbation. This latter assumption is satisfied by certain pseudo differential perturbations of a fixed differential operator but does not apply to paths of differential operators even in one dimension. As a result, the promising start made in [GLM+11] to generalising the Robbin-Salamon theorem (so that it applied to operators with some essential spectrum as occurs in the non-compact manifold case), ran into difficulties.

Subsequently, partial results (applicable to differential operators only in lower dimensions) have been obtained in the intervening years [CGL+16b], [CGLST16a], [CGG+16]. A significant advance that motivates this paper was made in the article [CGK16]. There, a trace formula is proved, again motivated by [BCP+06] and [GLM+11] (but by completely different methods than we employ here), that specialises under compact resolvent assumptions to give another version of the Robbin-Salamon theorem. More importantly however the formula applies even to situations where the operators considered are not Fredholm. It applies whether or not the operators in the path have zero in the essential spectrum. However, what is important is that in [CGK16] the trace formula was related to the spectral flow
only in the setting of unitarily equivalent endpoints with purely discrete spectra. We remove this restriction in this paper.

Relevant to the issue of allowing essential spectrum is that some time ago Witten [Wit82] gave a proposal for extending index theory beyond the Fredholm setting. For certain Dirac type operators (with essential spectrum) Witten’s ideas could be shown to produce index theorems [BGG+87, GS88]. Some of this early work also involves non-Fredholm operators and it was revisited in [CGP+17] and related to Pushnitski’s work under the same relative trace class assumption as in [GLM+11].

This led some of the present authors in [CGLS16a] to begin to complete the program started in [GLM+11]. The new ingredient in [CGLS16a] is an approximation technique that enabled the main theorems in [GLM+11] to be extended to more general examples where relatively trace class hypotheses were violated. It is this approximation technique that underpins the advances described in this paper.

Finally, further motivation for the present paper stems from attempts to use spectral flow in condensed matter theory, for example, [Sto96]. In this application Dirac type operators are used as Hamiltonians and spectral flow along paths of these operators provides information of physical interest. In some cases the operators in question are Fredholm with essential spectrum. Thus the Robbin-Salamon theorem does not apply. In other instances the paths of operators considered violate an important assumption in [RS95] namely, that the endpoints of the path of operators along which spectral flow is to be calculated are invertible. In this paper we are able to provide information on the spectral flow in this situation. We also mention that, in some examples using physical models, spectral flow is not well defined (as the operators in the path are not necessarily Fredholm). Our approach enables us to prove results in this non-Fredholm setting (see Theorem 8.12).

We summarise our point of view by remarking that whereas the Atiyah-Singer theorem [APS76] relates the analytical index to the spectral flow via the topological index our results express both the analytic index and the spectral flow in terms of quantities from quantum mechanical scattering theory. We note further that in the non-Fredholm situation that we study here we cannot necessarily expect topological formulas. This may be understood from the fact that in the non-Fredholm situation considered here we investigate properties modulo the trace class whereas the topological results follow because one works modulo compact operators. It is surprising nevertheless that we are able to replace the Fredholm index by the Witten index.

We make four main advances. First, our results are purely operator theoretic and hence apply in non-geometrical settings. Second in the setting of the Robbin-Salamon theorem we show that when one drops the assumption of invertible endpoints for the path one still obtains an index formula except that the Witten index replaces the Fredholm index. Third, we allow essential spectrum in the case of paths of self-adjoint Fredholm operators. Fourth, we show that we obtain information even in the case where the path of self-adjoint operators is not Fredholm. It is in this final situation that substantial results from quantum mechanical scattering theory are essential.

1.2. An overview of our results. We now briefly discuss the setting and results of the present paper and defer the discussions of methods and applications to the following section. For the purpose of an accessible introduction we consider here a simplified situation of the general setting under which we prove the results.
We start with a self-adjoint unbounded operator $A_-$ densely defined on a separable complex Hilbert space $\mathcal{H}$ and suppose that $B$ is a self-adjoint bounded perturbation of $A_-$. If the perturbation $B$ is a relative trace-class perturbation of $A_-$, that is, $B(A_- + i)^{-1}$ is a trace-class operator, then the main assumption in [GLM+11], [CGP+17] is satisfied. Hence, the results summarised in the previous subsection are known to be true. However, the critical fact for partial differential operators in general is that perturbations by lower order operators satisfy relative Schatten–von Neumann class constraints but not relative trace class constraints.

To describe this, suppose for example that we consider Schatten–von Neumann class constraints but not relative trace class constraints. The only way that we know of to obtain a relative trace class perturbation in dimensions is to replace $M$ by Dirac type operators on certain non-compact manifolds (see [CGRS14]). See Section 10 below for the example of the Dirac operator on $\mathbb{R}^2$, $d \in \mathbb{N}$.

To discuss the connection to index theory, we introduce now the ‘suspension’ operator $D_A$ as in [APS76], [RS95]. Let $\theta : \mathbb{R} \to \mathbb{R}$ be a smooth function (with integrable positive derivative) interpolating between zero and one in the sense that $\lim_{t \to -\infty} \theta(t) = 0$ and $\lim_{t \to \infty} \theta(t) = 1$. Denoting by $M_{\theta}$ the operator on $L^2(\mathbb{R})$ of multiplication by $\theta$, we introduce the operator $D_A$ in the Hilbert space $L^2(\mathbb{R}) \otimes \mathcal{H}$ by

\begin{equation}
D_A = \frac{d}{dt} \otimes 1 + 1 \otimes A_- + M_{\theta} \otimes B.
\end{equation}

Here the operator $d/dt$ in $L^2(\mathbb{R})$ is the differentiation operator with domain being the Sobolev space $W^{1,2}(\mathbb{R})$, so that $D_A$ is defined on $W^{1,2}(\mathbb{R}) \otimes \text{dom}(A_-)$. For ease of notation we will usually identify $L^2(\mathbb{R}) \otimes \mathcal{H}$ and $L^2(\mathbb{R}; \mathcal{H})$.

In order to relate the index theory of the operator $D_A$ with the spectral flow (when defined) of the family $\{A_- + \theta(t)B\}_{t \in \mathbb{R}}$ we establish firstly the first primary result of this current paper, the principal trace formula. Namely, under some additional mild assumptions for any $t > 0$ we prove the following relation (see Theorem 6.4 below):
\begin{align}
\text{tr} \left( e^{-tD^*_A D_A} - e^{-tD^*_A D_A} \right) &= -\left( \frac{t}{\pi} \right)^{1/2} \int_0^1 \text{tr} \left( e^{-tA_s^2} B \right) ds,
A_s &= A_- + sB, \quad s \in [0,1],
\end{align}

noting that our hypotheses guarantee both sides of the relation are well-defined. Here, \text{tr} denotes the classical trace on the algebra \( \mathcal{B}(\mathcal{H}) \) of all bounded linear operator on a Hilbert space \( \mathcal{H} \).

The key point to note is that this is an operator identity that makes no assumptions on the spectrum of the operators on either side of the relation. One of our key objectives is to develop the consequences of this fact, principally by using scattering theory methods. We discuss these methods in the next section.

We note that if we impose the assumption that the operators \( A_- \) and \( A_+ := A_- + B \) have discrete spectrum and are unitarily equivalent and invertible then the operators \( A_\pm \) and \( D_A \) are Fredholm and in that case the left-hand side of \((1.2)\) is the Fredholm index of \( D_A \) \cite{GS88} while the right hand side is the spectral flow along the path \( \{ A_- + \theta(t) B \}_{t \in \mathbb{R}} \). Thus the principal trace formula entails a version of the Robbin-Salamon theorem.

However, if we assume that the endpoints \( A_\pm \) are not invertible, the principal trace formula remains true, but the left-hand side is no longer the Fredholm index since the operator \( D_A \) is no longer Fredholm. However the right-hand side will still be spectral flow if \( A_\pm \) have discrete spectrum. As the right-hand side is independent of \( t \) in this case \cite{CP04} so too is the left-hand side and as discussed below, it is the Witten index of \( D_A \).

If the operator \( A_- \) has some essential spectrum then neither the left hand side nor the right hand side of the principal trace formula can be proved to be independent of \( t \). There are then two possible asymptotic quantities that we might consider. The first, the limit as \( t \to 0 \) on the left-hand side of the principal trace formula, gives what has been referred to in the physics literature as the anomaly. In the context of the Atiyah-Singer index theorem it gives the local form of the theorem involving integrals of characteristic classes. There is evidence \cite{CGK15} that for Dirac type operators with some essential spectrum the anomaly can be expressed in terms of a local formula of the same type as arises in the Atiyah-Singer theorem.

Our main interest in the present paper lies in the second limit as \( t \to \infty \) of \((1.2)\). On the left hand side this limit, if it exists, has been termed the Witten index \cite{GS88}. In the case of the right-hand side this limit has not been previously investigated. We provide here arguments that allow us to regard this limit of the right-hand side as a generalisation of spectral flow to the non-Fredholm setting. In particular, if the endpoints \( A_\pm \) are Fredholm operators, this generalised spectral flow gives the classical spectral flow.

The study of the limit \( t \to \infty \) in the principal trace formula is made possible by exploiting the Krein spectral shift function from quantum mechanical scattering theory. That is, both limits are computed by the respective spectral shift functions. We remark here that a number of applications of the principal trace formula are made in this paper including to a generalisation of the original formulas of Pushnitski relating the spectral shift function for the pair \((A_+, A_-)\) with that for the pair \((D_A^* D_A, D_A D_A^*)\). We also obtain results for the Witten index, and for spectral flow and its generalisations. These we now elaborate upon.
1.3. **Discussion of the methods and the applications.** The principal trace formula \([12]\) is an operator theoretic identity that makes no Fredholm type assumptions on the operators in question. For this reason it may be used to obtain information when the model operator \(DA\) is non-Fredholm. We will make use of the ideas that were previously introduced in \([CGP+17]\). In that paper the model operator \(DA\) in \(L^2(\mathbb{R}; \mathcal{H})\) was studied without Fredholm assumptions.

In this setting we replace the Fredholm index by the so-called Witten index. Recall \([GS88]\) that the semigroup (heat kernel) regularized Witten index, denoted \(Ws(DA)\), of the operator \(DA\) is defined by

\[
Ws(DA) = \lim_{t \to \infty} \text{tr}_\mathcal{H} (e^{-tDA^*DA} - e^{-tDA^*DA}),
\]

whenever the limit exists.

In the particular case, when the operator \(DA\) is Fredholm, one has consistency with the Fredholm index, \(\text{index}(DA)\) of \(DA\) \([GS88]\), that is,

\[
\text{index}(DA) = Ws(DA).
\]

There is also a resolvent regularised Witten index described in \([BGG+87], [CGP+17]\) and references therein, introduced via the difference of resolvents of \(DA^*DA\) and \(DA^*DA\). However, in the setting of differential operators on higher dimensional manifolds this difference is typically not a trace-class operator. Hence, following \([CGK15]\), we introduced \(k\)-th resolvent regularised Witten index \(W_{k,r}(DA)\) of \(DA\) by setting

\[
W_{k,r}(DA) = \lim_{\lambda \to 0} (-\lambda)^k \text{tr} ((DA^*DA - \lambda)^{-k} - (DA^*DA - \lambda)^{-k})
\]

whenever this limit exists. In the terminology of \([CGK15]\) this is the limit as \(\lambda \uparrow 0\) of the homological index of \(DA\).

In general (i.e., if \(DA\) is not Fredholm), \(Ws(DA)\) is not necessarily integer-valued; in fact, one can show that it can take on any prescribed real number. The intrinsic value of \(Ws(DA)\) then lies in its stability properties with respect to additive perturbations, analogous to stability properties of the Fredholm index. Indeed, as long as one replaces the familiar relative compactness assumption on the perturbation in connection with the Fredholm index, by appropriate relative trace class conditions in connection with the Witten index, stability of the Witten index was proved in \([BGG+87]\) and \([GS88]\).

We will not go over the extensive history associated with the Witten index but refer the reader to \([CGP+17]\) for a full bibliography. We remark however that there is evidence that in geometric situations the Witten index is connected to the geometry of the manifold at infinity.

As can be seen from the definition of the semigroup regularised Witten index \(Ws(DA)\) and the principal trace formula \([12]\), we can compute \(Ws(DA)\) by taking the limit of the right-hand side of principal trace formula as \(t \to \infty\). To describe this limit we use methods of scattering theory, namely the spectral shift function of M.G. Krein. For a full exposition of the theory of Krein’s spectral shift function we refer to \([Yaf92, Section 8]\) while for those aspects relevant to this article there is the review \([CGLS16b]\).

The spectral shift function was introduced by M.G. Krein in \([Kre53]\), who was inspired by results of Lifshitz on Hamiltonians of a lattice model in quantum mechanics. Krein proved that for two self-adjoint operators \(H\) and \(H_0\) with common
domain and the perturbation $H - H_0$ of trace-class, there exists a unique (Lebesgue) integrable function $\xi(\cdot; H, H_0)$ on $\mathbb{R}$ satisfying the so-called Lifshitz-Krein trace formula
\[ \text{tr} \left( f(H) - f(H_0) \right) = \int_{\mathbb{R}} f'(\lambda) \xi(\lambda; H_0, H_0 + V) d\lambda, \]
for a large class of functions $f$.

Krein’s work can be applied (with some further definitions that we omit for the purposes of this introductory discussion) to the operators introduced above, that is, to the pairs of operators $(A_+, A_-)$ and $(D_A^* D_A, D_A D_A^*)$. Hence, using the Lifshitz-Krein trace formula for the left-hand side of principal trace formula (1.2) we can write
\[ \text{tr}(e^{-tD_A^* DA} - e^{-tDA^* D_A}) = -t \int_{0}^{\infty} \xi(\lambda; D_A^* D_A, D_A D_A^*) e^{-t\lambda} d\lambda. \]
That is, the left-hand side of the principal trace formula can be rewritten as the Laplace transform of the spectral shift function $\xi(\cdot; D_A^* D_A, D_A D_A^*)$.

For the right-hand side of the principal trace formula, the Lifshitz-Krein trace formula can not be used directly. However, exploiting results from [CGL+16a], we prove the equality
\[ \int_{0}^{1} \text{tr} \left( e^{-tA^2} (A_+ - A_-) \right) ds = \int_{0}^{\infty} \xi(s, A_+, A_-) e^{-ts^2} ds, \quad t > 1, \]
and therefore, as a corollary of the principal trace formula, the uniqueness theorem for the Laplace transform and its simple properties we conclude that the spectral shift functions $\xi(\cdot; D_A^* D_A, D_A D_A^*)$ and $\xi(\cdot; A_+, A_-)$ are related via a so-called Pushnitski formula (see Theorem 7.3 below)
\[ \xi(\lambda; D_A^* D_A, D_A D_A^*) = \frac{1}{\pi} \int_{\lambda - \lambda^2 / 2}^{\lambda + \lambda^2 / 2} \frac{\xi(\nu; A_+, A_-) d\nu}{(\lambda - \nu^2)^{1/2}}, \quad \text{a.e. } \lambda > 0, \]
which generalises [Pus08] and [GLM+11].

Pushnitski’s formula together with some Tauberian theorems allows us to establish the first of the applications of the present paper. It relates the Witten index of the operator $D_A$ with the value at zero (in a Lebesgue sense) of the spectral shift function $\xi(\cdot; A_+, A_-)$. We use the notation $\xi_L(0_+; A_+, A_-)$ and $\xi_L(0_-; A_+, A_-)$, respectively, to denote the left and right hand value of $\xi(\cdot; A_+, A_-)$ at zero in the sense of Lebesgue.

**Theorem 1.1.** Assume Hypothesis [75]. Assume that 0 is a right and a left Lebesgue point of $\xi(\cdot; A_+, A_-)$. Then the semigroup regularised Witten index $W_s(D_A)$ as well as the $k$-th resolvent regularised index $W_{k,r}(D_A)$ exist for sufficiently large $k \in \mathbb{N}$ and equal
\[ W_s(D_A) = W_{k,r}(D_A) = \frac{[\xi_L(0_+; A_+, A_-) + \xi_L(0_-; A_+, A_-)]}{2}. \]  

As one-dimensional examples show [CGL+16b, CGG+10], the equality in Theorem 1.1 holds even in the case when the endpoints $A_{\pm}$ have purely absolutely continuous spectra coinciding with the whole real line. Our preliminary investigation of multidimensional examples demonstrates that, in many cases, the spectral shift function $\xi(\cdot; A_+, A_-)$ is sufficiently regular at zero for the abstract analysis of this paper to apply, and therefore, equality 1.3 holds. However, we defer a full exposition of this fact as the arguments are long and technical.
As shown in \[\text{ACS07}\] for operators $A_{\pm}$ with compact resolvent (in the sense of general semifinite von Neumann algebras), the spectral shift function $\xi(\cdot; A_{+}, A_{-})$ at zero is equal to the spectral flow up to kernel correction terms. However, for our primary example of Dirac operators on $\mathbb{R}^d$, the operators $A_{\pm}$ do not have compact resolvent. Thus, in our setting, \[\text{ACS07}\] is not applicable.

Nevertheless, in the case when the endpoints $A_{\pm}$ are Fredholm and for a suitable path \{\(A(t)\)\}_{t \in \mathbb{R}} joining $A_{+}$ and $A_{-}$, we prove that the spectral flow for \{\(A(t)\)\}_{t \in \mathbb{R}} defined using the analytic approach of \[\text{Phi96}\], is again equal to the value of the spectral shift function $\xi(\cdot; A_{+}, A_{-})$ at zero modulo the correction terms. In particular, employing Theorem 1.1 we obtain the following generalisation of the Robbin-Salamon formula.

**Theorem 1.2.** Assume Hypothesis 5.1 and assume, in addition, that the endpoint $A_{\pm}$ are Fredholm operators. Then the spectral flow $\text{sf}(\{A(t)\}_{t \in \mathbb{R}})$ along the path \{\(A(t)\)\}_{t \in \mathbb{R}} exists, the Witten index $W_{s}(D_{A})$ of the operator $D_{A}$ exists and we have the equality

$$W_{s}(D_{A}) = \text{sf}(\{A(t)\}_{t \in \mathbb{R}}) - \frac{1}{2}(\dim(\ker(A_{+})) - \dim(\ker(A_{-}))).$$

In the particular case, when the path \{\(A(t)\)\}_{t \in \mathbb{R}} consists of operators with purely discrete spectra and the endpoints are unitarily equivalent we recover a version of the result of \[\text{RS95}\]. Interestingly though, our formula generalises also results of \[\text{Pus08}\] and \[\text{GLM+11}\]. We also note \[\text{CGP+15}\], in which it is shown that for unitarily equivalent endpoints, where the unitary satisfies additional constraints, one may obtain a residue formula for spectral flow between $A_{\pm}$. The limiting process used there is analogous in some ways to the limiting process we use here in that we take the parameter $t$ in the principal trace formula to infinity.

This extension of previous results to the case where $A_{-}$ is Fredholm, but there are no restrictions on the kernels of either $A_{-}$ or $A_{+}$, is likely to have applications in condensed matter theory. We have in mind models of, for example, topological phases of matter, where $A_{\pm}$ are Hamiltonians and the case where they have kernels is precisely the most interesting one.

Now we turn to the case where $A_{\pm}$ need not be Fredholm. This puts us outside existing theory except for \[\text{CGP+17}\] and \[\text{CGLS16b}\] where relatively trace class perturbation assumptions are made. There are several new results in this paper pertaining to this case. The most important of these is the principal trace formula (1.2) itself.

In the non-Fredholm setting, the left-hand side of the principal trace formula leads to the Witten index. Hence, a natural question is to ask what the right-hand side of the principal trace formula represents in the non-Fredholm case. In the absence of compact resolvent assumptions our ideas are inspired by an old example of one of us (ALC) and Harald Grosse that may be found in an unpublished manuscript having its roots in investigations of gauge transformations in fermionic quantum field theories in the 1980s \[\text{CHO82}\]. We described the example in \[\text{CGG+16}\]. This example suggested to us that the limit of the right-hand side of the principal trace formula as $t \to \infty$, when it exists, is a generalisation of spectral flow to the non-Fredholm situation just as the Witten index generalises the Fredholm index.

However, to show that this limit of the right-hand side of the principal trace formula can be regarded as generalised spectral flow, we have to establish some
properties of the integral

$$\int_0^1 \text{tr} \left( e^{-t A_s^2} B \right) ds, \quad A_s = A_- + sB, \quad t > 0$$

on the right-hand side of the principal trace formula. For the path of Fredholm operators (with a certain smoothness condition), it is known that the integral in (1.4) represents the integral formula for the spectral flow \([CP98]\). Since the spectral flow is a homotopy invariant of the space of Fredholm operators, by analogy, we obtain here a weakened form of homotopy invariance for the integral (1.4). We prove that in general this integral is independent of the choice of sufficiently smooth path joining \(A_-\) as long as this path remains in an affine space of ‘admissible’ perturbations (we make this notion precise later, see Section 9). Our proof is an extension of ideas from \([CPS09]\). What we prove is that the integrand in (1.4) is an exact one form on our affine space of admissible perturbations regarded as a Banach manifold.

**Theorem 1.3.** Let \(A_-\) be a self-adjoint operator and let \(B\) be a \(p\)-relative trace class perturbation of \(A_-\). The integral

$$\lim_{t \to \infty} \left[ -\left( \frac{1}{\pi} \right)^{1/2} \int_0^1 \text{tr} \left( e^{-t A_s^2} (A_+ - A_-) \right) ds \right]$$

does not depend on a smooth path \(\{A_s\}_{s \in [0,1]}\) in the affine space of \(p\)-relative trace-class perturbations of \(A_-\), joining \(A_-\) and \(A_- + B\).

The result above suggests that in the non-Fredholm case we can relate

$$\lim_{t \to \infty} \left[ -\left( \frac{1}{\pi} \right)^{1/2} \int_0^1 \text{tr} \left( e^{-t A_s^2} (A_+ - A_-) \right) ds \right]$$

to a generalisation of spectral flow along an admissible path joining \(A_\pm\) when \(A_\pm\) are unitarily equivalent. One consequence of this paper is that when the Witten index exists so too does the limit on the right-hand side. Then by inserting kernel correction terms on the right-hand side we obtain a notion of generalised spectral flow when the endpoints \(A_\pm\) are not invertible.

Moreover under appropriate regularity assumptions of the respective spectral shift functions at zero we see that generalised spectral flow can be expressed in terms of the spectral shift function just as in the Fredholm case. This fact may have applications in condensed matter theory where variations in parameters in the Hamiltonian can result in the closing of the spectral gap at zero.

### 1.4. Summary of the exposition.

In Section 2 we collect some preliminaries. In order to make our text more self contained we give an exposition of the main tool that we use, namely double operator integrals (DOI) in Section 2.1. This technique has had many applications in non-commutative analysis in the last few years and we intend our exposition in this paper to be useful in other contexts.

Following this in Section 3 we give a detailed exposition of the setting and explain the approximation scheme that we use in order to apply the results of \([Pus08, GLM+11]\). The idea is to use a ‘cut-off’ that, in the case of differential operators, produces a sequence of pseudo-differential approximants. This is the technical heart of the paper. The point is that for the approximants the principal trace formula is quickly established. Then in Section 6 we have to handle the convergence of both sides as we remove our cut-off thus proving the principal trace formula.
The rest of the paper is about applications. In Section 7 we firstly introduce the spectral shift function adapted to our setting. There is a subtle point that we need to be careful about in that for the pair \( A_\pm \) the spectral shift function is a priori only defined up to a constant. Fixing this constant is essential but is not a trivial matter. With these preliminaries out of the way we move to our analogue of Pushnitski's formula. Then we discuss the Witten index.

Next, in Section 8 comes our discussion of how to obtain a version of the Robin-Salamon theorem for Fredholm operators with some essential spectrum. Here we also discuss the non-Fredholm case. We argue that the principal trace formula suggests a definition of ‘generalised spectral flow’ for paths of non-Fredholm operators. We then present some basic properties of this generalised spectral flow. We prove that the right-hand side of the principal trace formula is the integral of an exact one form on the space of admissible perturbations of \( A_- \) leading to restricted homotopy invariance.

The final Section is devoted to examples. The main results are about Dirac operators in arbitrary dimensions. We sketch some work in progress that is relevant to the regularity issue that arises for the spectral shift function in earlier Sections. We give explicit examples of the general operator theoretic formalism developed earlier.

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1.5. Notation. For a Banach space \( \mathcal{X} \) we denote by \( B(\mathcal{X}) \) the algebra of all linear bounded operators on \( \mathcal{X} \).

In case when \( \mathcal{X} = \mathcal{H} \) is a separable complex Hilbert space \( \mathcal{H} \), we use notation \( \| \cdot \| \) for the uniform norm. The corresponding \( \ell^p \)-based Schatten–von Neumann ideals on \( \mathcal{H} \) are denoted by \( \mathcal{L}_p(\mathcal{H}) \), with associated norm abbreviated by \( \| \cdot \|_p, p \geq 1 \). Moreover, \( \text{tr}(A) \) denotes the trace of a trace class operator \( A \in \mathcal{L}_1(\mathcal{H}) \).

We use symbols \( n\text{-lim} \) and \( s\text{-lim} \) to denote the operator norm limit (i.e., convergence in the topology of \( B(\mathcal{H}) \)), and the operator strong limit.

If \( T \) is a linear operator mapping (a subspace of) a Hilbert space \( \mathcal{H} \) into another, then \( \text{dom}(T) \) and \( \text{ker}(T) \) denote the domain and kernel (i.e., null space) of \( T \). The closure of a closable operator \( S \) is denoted by \( \overline{S} \). The spectrum and resolvent set of a closed linear operator in \( \mathcal{H} \) will be denoted by \( \sigma(\cdot) \), and \( \rho(\cdot) \), respectively.

The notation \([\cdot, \cdot]\) stands for commutator of two operators, that is

\[ [A, B] = AB - BA. \]
The space of all Schwartz function on $\mathbb{R}^d$ is denoted by $S(\mathbb{R}^d)$ and the Sobolev spaces are denoted by $W^{p,q}(\mathbb{R}^d)$. Unless explicitly stated otherwise, whenever we write $L_p(\mathbb{R}^d)$ ($L_p(0, \infty)$ etc.) we assume the classical Lebesgue measure on $\mathbb{R}^d ((0, \infty)$ etc.).

By $L^2(\mathbb{R}, \mathcal{H})$ we denote the Hilbert space of all $\mathcal{H}$-valued Bochner square integrable function on $\mathbb{R}$. Linear operators in the Hilbert space $L^2(\mathbb{R}; \mathcal{H})$, will be denoted by calligraphic boldface symbols of the type $\mathcal{T}$, to distinguish them from operators $T$ in $\mathcal{H}$. In particular, operators denoted by $\mathcal{T}$ in the Hilbert space $L^2(\mathbb{R}; \mathcal{H})$ typically represent operators associated with a family of operators $\{T(t)\}_{t \in \mathbb{R}}$ in $\mathcal{H}$, defined by

$$(Tf)(t) = T(t)f(t) \text{ for } \text{a.e. } t \in \mathbb{R},$$

(1.5) \quad $f \in \text{dom}(\mathcal{T}) = \{g \in L^2(\mathbb{R}; \mathcal{H}) \mid g(t) \in \text{dom}(T(t)) \text{ for } \text{a.e. } t \in \mathbb{R};$

\[ t \mapsto T(t)g(t) \text{ is (weakly) measurable; } \int_{\mathbb{R}} \|T(t)g(t)\|_{\mathcal{H}}^2 \, dt < \infty \}. \]

We denote by $[\cdot]$ the floor function on $\mathbb{R}$ (that is, $[x]$ is the largest integer which is less than or equal $x \in \mathbb{R}$) and for a real number $x \in \mathbb{R}$ the notation $\{x\}$ stands for the fractional part of $x$ given by $x - [x]$. Finally, we employ the abbreviations

$$g_+(x) = x(x^2 - z)^{-1/2}, \quad z \in \mathbb{C}\setminus[0, \infty), \quad g(x) = g_{-1}(x), \quad x \in \mathbb{R}. $$

### 2. Preliminaries

In the present section we present the main technical tool of our approach: namely double operator integrals (DOI) and introduce the class of so-called $p$-relative trace class perturbations of a given self-adjoint operator. This class of perturbations constitutes the essential part of the main hypothesis for our central results (see Hypothesis 3.1). We introduce this class in Section 2.2 where we collect all the preliminary properties of $p$-relative trace-class perturbations.

#### 2.1. Double operator integrals.

In this section we introduce a technical tool of double operator integrals, which is the main tool in the proof of the Principal trace formula (see Theorem 6.4). We refer the reader to [BS06, BS07, BS73, PS09, PS08] for the precise definition of double operator integrals and their properties (see also the survey [BS03]).

Let $\mathcal{H}$ be a Hilbert space, suppose the $A_0, A_1$ are self-adjoint operators acting on $\mathcal{H}$, and $f$ is a bounded Borel function on $\sigma(A_0) \times \sigma(A_1)$. Heuristically, the **double operator integral** $T_f^{A_0, A_1}$ is a mapping acting on $\mathcal{B}(\mathcal{H})$ and is defined using the spectral measures $E_{A_0}$ and $E_{A_1}$ of $A_0$ and $A_1$ by

$$T_f^{A_0, A_1}(B) := \int_{\sigma(A_1)} \int_{\sigma(A_0)} f(\lambda, \mu) \, dE_{A_0}(\lambda) B \, dE_{A_1}(\mu), \quad B \in \mathcal{B}(\mathcal{H}).$$

For a given function $f$ on $\sigma(A_0) \times \sigma(A_1)$, the double operator integral $T_f^{A_0, A_1}$ may or may not be a bounded operator on $\mathcal{B}(\mathcal{H})$ (or on normed ideals of $\mathcal{B}(\mathcal{H})$). We note (see e.g. [BS03, Section 4.1]) that a double operator integral $T_f^{A_0, A_1}$ is bounded on $\mathcal{B}(\mathcal{H})$ if and only if the double operator integral $T_f^{A_0, A_1}$ is bounded on $\mathcal{L}_1$, where $\bar{f}$ is the complex conjugate of $f$.  


Recall that for a differentiable function $h : [0, 1] \to \mathbb{C}$, the divided difference $h^{[1]}$ is the function on $\mathbb{R}^2$ defined by

$$h^{[1]}(\lambda, \mu) = \begin{cases} \frac{h(\lambda) - h(\mu)}{\lambda - \mu}, & \text{if } \lambda \neq \mu, \\ h'(\lambda), & \text{if } \lambda = \mu, \end{cases} \quad \lambda, \mu \in \mathbb{R}.$$ 

Define the function

$$\phi(\lambda, \mu) = (\lambda^2 + 1)^{1/4} \cdot g^{[1]}(\lambda, \mu) \cdot (\mu^2 + 1)^{1/4}, \tag{2.1}$$

where $g$ is defined by (L0).

**Lemma 2.1.** [GLM+11] Lemma 6.6] Suppose that $A, B$ are self-adjoint operators such that $A - B \in L^p(\mathcal{H})$, $1 \leq p < \infty$. The double operator integral $T_{\phi}^{A,B}$ with function $\phi$ defined by (2.1) is bounded on $L^p(\mathcal{H})$, $1 \leq p < \infty$, and on $\mathcal{B}(\mathcal{H})$ and

$$g(A) - g(B) = T_{\phi}^{A,B}((A^2 + 1)^{-1/4}(A - B)(B^2 + 1)^{-1/4}).$$

The following proposition provides an easy corollary of the Daletski-Krein formula (see e.g. [BS73]). We refer also to [Sim98].

**Proposition 2.2.** Let $A$ be a self-adjoint operator acting in a separable Hilbert space $\mathcal{H}$, $B \in \mathcal{L}_1(\mathcal{H})$ and let $f \in C_0^\infty(\mathbb{R})$ be such that $f' \in L^p(\mathbb{R})$ for some $p \geq 1$. Then, letting $A_s = A + sB$, $s \in [0, 1]$, we have that

$$\text{tr}(f(A_1) - f(A_0)) = \int_0^1 \text{tr}(f'(A_s)B)ds. \tag{2.2}$$

Next we recall results of [Yaf05] and [CGL+16]. Note that these result hold for significantly wider class of functions. For the purpose of the present paper, the class of Schwartz functions suffices.

**Proposition 2.3.** [Yaf05] Let $A, B$ be self-adjoint operators. Assume that for some odd $m \in \mathbb{N}$ for all $a \in \mathbb{R} \setminus \{0\}$, we have

$$[(B - ai)^{-m} - (A - ai)^{-m}] \in \mathcal{L}_1(\mathcal{H}) \tag{2.3}$$

and let $f \in S(\mathbb{R})$. Then there exist double operator integrals $T_{f,a_i}^{A,B}$ and $T_{f,a_2}^{A,B}$, which are bounded on $\mathcal{L}_1(\mathcal{H})$ and

$$f(A) - f(B) = \sum_{j=1}^2 T_{f,a_j}^{A,B}((A - a_ji)^{-m} - (B - a_ji)^{-m}) \in \mathcal{L}_1(\mathcal{H}).$$

**Theorem 2.4.** [CGL+16] Section 3] Assume that $A, A_n, B, B_n, n \in \mathbb{N}$, are self-adjoint operators such that $A_n \to A$ and $B_n \to B$ as $n \to \infty$ in the strong resolvent sense. In addition we assume that for some $m \in \mathbb{N}$, $m$ odd, and every $a \in \mathbb{R} \setminus \{0\}$,

$$[(A + ia)^{-m} - (B + ia)^{-m}], \ [(A_n + ia)^{-m} - (B_n + ia)^{-m}] \in \mathcal{L}_1(\mathcal{H}),$$

and

$$\lim_{n \to \infty} \|[(A_n + ia)^{-m} - (B_n + ia)^{-m}] - [(A + ia)^{-m} - (B + ia)^{-m}]\|_1 = 0. \tag{2.4}$$
Then for any \( f \in S(\mathbb{R}) \) and the double operator integrals \( T_{f,\alpha_j}^{A,B} \) and \( T_{f,\alpha_j}^{A,B_n} \) as in Proposition 2.3 we have that
\[
T_{f,\alpha_j}^{A,B_n} \to T_{f,\alpha_j}^{A,B}, \quad j = 1, 2,
\]
pointwise on \( L_1(\mathcal{H}) \). In particular,
\begin{equation}
\lim_{n \to \infty} \left\| [f(A_n) - f(B_n)] - [f(A) - f(B)] \right\|_{L_p(\mathcal{H})} = 0.
\end{equation}

2.2. The class of \( p \)-relative trace class perturbations. In this section we introduce the class of perturbations needed for the rest of the present paper.

**Definition 2.5.** Let \( A_0 \) be a self-adjoint operator on a separable Hilbert space \( \mathcal{H} \) and let \( p \in \mathbb{N} \cup \{0\} \). A bounded self-adjoint operator \( B \in \mathcal{B}(\mathcal{H}) \) is called a \( p \)-relative trace class perturbation (with respect to \( A_0 \)) if
\begin{equation}
B(A_0 + i)^{-p-1} \in L_1(\mathcal{H}).
\end{equation}
In what follows, we choose the smallest \( p \), such that (2.6) holds.

It is clear that one can take the resolvent parameter for the operator \( A_0 \) to be any point \( z \in \mathbb{C} \setminus \mathbb{R} \) for the definition of \( p \)-relative trace class perturbations. In addition, since \( B \) is self-adjoint, inclusion (2.6) is equivalent to the inclusion \( (A_0 + i)^{-p-1} B \in L_1(\mathcal{H}) \).

**Remark 2.6.** The fact that the function \( f(t) = \frac{(t+i)^q}{(t^2+1)^{q/2}}, \ t \in \mathbb{R}, \ q \in \mathbb{R} \), is bounded together with its reciprocal, implies that for any \( C \in \mathcal{B}(\mathcal{H}) \) the operators
\[
C(A_0 + i)^{-q} \quad \text{and} \quad C(A_0^2 + 1)^{-q/2}
\]
belong to the same ideal of \( \mathcal{B}(\mathcal{H}) \). In what follows we use this fact repeatedly without additional explanations.

Classical interpolation theory for Schatten ideals (see see e.g. [Sim05, Theorem 2.9], [GK69, Section III, Theorem 13.1]) implies the following simple result.

**Lemma 2.7.** Suppose that \( B \) is a \( p \)-relative trace-class perturbation of \( A_0 \). Then
\begin{enumerate}
\item[(i)] For any \( j = 1, \ldots, p+1 \), we have
\begin{equation}
B(A_0 + i)^{-j} \in L_{\frac{p+1}{j+1}}(\mathcal{H}), \quad j = 1, \ldots, p+1,
\end{equation}
and
\begin{equation}
\|B(A_0 + i)^{-j}\|_{L_{\frac{p+1}{j+1}}} \leq \|B\|_{L_{p+1}} \cdot \|B(A_0 + i)^{-p-1}\|_{L_1}^{\frac{p+1-j}{p+1}}.
\end{equation}

\item[(ii)] For any \( j = 1, \ldots, p+1 \) and any \( k,l \in \mathbb{N} \cup \{0\} \) such that \( k+l = j \), we have
\[
(A_0 + i)^{-k}B(A_0 + i)^{-l} \in L_{\frac{p+1}{j+1}}(\mathcal{H}).
\]
and
\begin{equation}
\|(A_0 + i)^{-k}B(A_0 + i)^{-l}\|_{L_{\frac{p+1}{j+1}}} \leq \|B(A_0 + i)^{-j}\|_{L_{\frac{p+1}{j+1}}}^{\frac{p+1-j}{p+1}}.
\end{equation}
\end{enumerate}

**Proof.** (i). Consider the operator-valued function \( T(z) = B(A_0^2+1)^{\frac{(p+1)(j-1)}{2}} \) defined in the strip \( 0 \leq \text{Re}(z) \leq 1 \). By assumption, we have
\[
T(it) = B(A_0^2 + 1)^{-\frac{p+1}{2}} \cdot (A_0^2 + 1)^{-it\frac{p+1}{2}} \in L_1(\mathcal{H})
\]
and
\[
T(1+it) = B \cdot (A_0^2 + 1)^{-it\frac{p+1}{2}} \in \mathcal{B}(\mathcal{H}).
\]
Hence, an application of three lines theorem (see e.g. [Sim05, Theorem 2.9], [GK69, Section III, Theorem 13.1]) yields the required result with \( \text{Re}(z) = \frac{p+1}{p+1} \).

The second assertion of the lemma can be proved similarly (see also [GLST15]). □

Inclusion (2.7) combined with Weyl’s theorem (see e.g. [Wei80, Theorem 9.13]) implies the stability of essential spectra, a classical result, which we state separately for convenience.

**Proposition 2.8.** Suppose that \( B \) is a \( p \)-relative trace-class perturbation of \( A_0 \). Then

\[
\sigma_{\text{ess}}(A_0 + B) = \sigma_{\text{ess}}(A_0).
\]

Next, we shall show that the assumption that \( B \) is a \( p \)-relative trace class perturbation of a self-adjoint operator \( A_0 \), guarantees that \((A_0 + B - ai)^{-p} - (A_0 - ai)^{-p}\) is a trace-class operator. In addition, we establish an approximation result for the difference \((A_0 + B - ai)^{-p} - (A_0 - ai)^{-p}\) necessary for the proof of the principal trace formula.

Firstly, we recall a result which is used repeatedly throughout the paper. This result can be found in [Sim05] and [GLM11, Lemma 3.4].

**Lemma 2.9.** Let \( p \in [1, \infty) \) and assume that \( R, R_n, T, T_n \in \mathcal{B}(\mathcal{H}), n \in \mathbb{N} \), satisfy

\[
s\lim_{n \to \infty} R_n = R, \quad s\lim_{n \to \infty} T_n = T
\]

and that \( S, S_n \in L_p(\mathcal{H}), n \in \mathbb{N} \), satisfy \( \lim_{n \to \infty} \|S_n - S\|_p = 0 \). Then \( \lim_{n \to \infty} \|R_n S_n T_n^* - RST^*\|_p = 0 \).

We now introduce special spectral ‘cut-off’ approximants \( B_n, n \in \mathbb{N} \), for a \( p \)-relative trace-class perturbation \( B \).

**Definition 2.10.** Let \( A_0 \) be a self-adjoint operator in \( \mathcal{H} \) and let \( B \) be a \( p \)-relative trace-class perturbation of \( A_0 \). For every \( n \in \mathbb{N} \) we introduce

\[
P_n = \chi_{[-n,n]}(A_0)
\]

and

\[
B_n := P_n BP_n.
\]

Throughout this section we will assume that \( P_n \) and \( B_n, n \in \mathbb{N} \), are as in the above definition.

It follows from spectral theory that

\[
s\lim_{n \to \infty} P_n = 1.
\]

We also note that the equality (2.6) together with the definition of the projections \( P_n \) implies that

\[
B_n = P_n BP_n \in L_1(\mathcal{H}).
\]

**Remark 2.11.** The precise form of the cut-offs \( P_n \) is of course immaterial. We just need several facts: that \( s\lim_{n \to \infty} P_n = 1 \), \( \sup_{n \in \mathbb{N}} \|P_n\| < \infty \) and that \( P_n BP_n \in L_1(\mathcal{H}) \).

The following lemma gathers some simple properties of the approximants \( A_0 + B_n, n \in \mathbb{N} \).
Lemma 2.12. Let $B$, $B_n$ and $P_n$ be as in Definition 2.10. We have that

(i) $A_0 + B_n \rightarrow A_0 + B$ in the strong resolvent sense as $n \rightarrow \infty$;

(ii) Let $j \in \mathbb{N}$. For any $k, l \in \mathbb{N}$ such that $k + l \geq j$ and $z \in \mathbb{C} \setminus \mathbb{R}$, we have

$$\lim_{n \rightarrow \infty} \left\|(A_0 - z)^{-k}B_n(A_0 - z)^{-l} - (A_0 - z)^{-k}B(A_0 - z)^{-l}\right\|_{\mathcal{L}(\mathcal{H})} = 0.$$ 

Proof. (i). Since the operator $B$ is bounded, it follows that the operators $A_0 + B_n$ and $A_0 + B$ have common core $\text{dom}(A_0)$. Therefore, by [RS80] Theorem VIII.25 (a) it is sufficient to show that $(A_0 + B_n)\xi \rightarrow (A_0 + B)\xi$ for all $\xi \in \text{dom}(A_0)$.

Let $\xi \in \text{dom}(A_0)$. Since $P_n \rightarrow 1$ in the strong operator topology, we have that $B_n\xi = P_nBP_n\xi \rightarrow B\xi$ for any $\xi \in \text{dom}(A_0)$. Hence

$$\|(A_0 + B_n)\xi - (A_0 + B)\xi\| = \|B_n\xi - B\xi\| \rightarrow 0, \quad \xi \in \text{dom}(A_0).$$

Thus, $A_0 + B_n \rightarrow A_0 + B$ in the strong resolvent sense.

(ii). Since $k + l \geq j$, Lemma 2.7 (ii) implies that

$$(A_0 - z)^{-k}B(A_0 - z)^{-l} \in \mathcal{L}_{\frac{1}{k+l}}(\mathcal{H}).$$

Therefore, since

$$(A_0 - z)^{-k}B_n(A_0 - z)^{-l} = P_n(A_0 - z)^{-k}B(A_0 - z)^{-l}P_n,$$

and $P_n \rightarrow 1$ in the strong operator topology, the assertion follows from Lemma 2.9. \hfill \Box

Now, let us fix $j = 1, \ldots, p$ and consider the difference

$$(A_0 + B - z)^{-j} - (A_0 - z)^{-j}.$$ 

Our next aim is to show that this operator belongs to a Schatten ideal $\mathcal{L}_q(\mathcal{H})$, with $q \geq 1$ chosen as small as possible. To lighten notations, we introduce

$$A_1 = A_0 + B.$$ 

Using the elementary identity

$$C_1^j - C_2^j = \sum_{k_0 + k_1 = j - 1} C_1^{k_0} [C_1 - C_2] C_2^{k_1}, \quad C_1, C_2 \in \mathcal{B}(\mathcal{H}), \quad j \in \mathbb{N},$$

and the resolvent identity we can write

$$(A_1 - z)^{-j} - (A_0 - z)^{-j}$$

$$\quad = \sum_{k_0 + k_1 = j - 1} (A_1 - z)^{-k_0} \left( (A_1 - z)^{-1} - (A_0 - z)^{-1} \right) (A_0 - z)^{-k_1}$$

$$\quad = \sum_{k_0 + k_1 = j - 1} (A_1 - z)^{-k_0 - 1} B(A_0 - z)^{k_1 - 1}.$$

Writing

$$(A_1 - z)^{-k_0 - 1} = (A_0 - z)^{-k_0 - 1} + (A_1 - z)^{-k_0 - 1} - (A_0 - z)^{-k_0 - 1})$$

$$(A_0 - z)^{-k_0 - 1} = (A_0 - z)^{-k_0 - 1} + (A_0 - z)^{-k_0 - 1} - (A_0 - z)^{-k_0 - 1})$$
and repeating the same argument for the second term on the right-hand side we obtain

\[(A_1 - z)^{-j} - (A_0 - z)^{-j}\]

\[= - \sum_{k_0+k_1=j-1} (A_0 - z)^{-k_0-1} B(A_0 - z)^{k_1-1} \]

\[- \sum_{k_0+k_1=j-1} (A_1 - z)^{-k_0-1} - (A_0 - z)^{-k_0-1} ]B(A_0 - z)^{k_1-1}\]

\[= - \sum_{k_0+k_1=j-1} (A_0 - z)^{-k_0-1} B(A_0 - z)^{k_1-1} \]

\[- \sum_{k_0+k_1+k_2=j-1} (A_1 - z)^{-k_0-1} B(A_0 - z)^{-k_1-1} B(A_0 - z)^{k_1-1}.\]

If, for arbitrary \(j = 1, \ldots, p, i \in \mathbb{N}, z \in \mathbb{C} \setminus \mathbb{R}\) and \(X_1, \ldots, X_i \in \mathcal{B}(\mathcal{H})\), we introduce the following operators

\[(2.14)\]

\[T_1^{(j)}(X_1) = \sum_{k_0+k_1=j} (A_0 - z)^{-k_0-1} X_1(A_0 - z)^{-k_1-1},\]

\[T_2^{(j)}(X_1, X_2) = \sum_{k_0+k_1+k_2=j} (A_0 - z)^{-k_0-1} X_1(A_0 - z)^{-k_1-1} X_2(A_0 - z)^{-k_2-1},\]

\[\ldots\]

\[T_i^{(j)}(X_1, \ldots, X_i)\]

\[= \sum_{k_0+\cdots+k_i=j} (A_0 - z)^{-k_0-1} X_1(A_0 - z)^{-k_1-1} \cdots X_i(A_0 - z)^{-k_i-1},\]

and

\[R_i^{(j)}(B; X_1, \ldots, X_i)\]

\[= \sum_{k_0+\cdots+k_i=j} (A_1 - z)^{-k_0-1} X_1(A_0 - z)^{-k_1-1} \cdots X_i(A_0 - z)^{-k_i-1},\]

then we have a Taylor formula for the difference \((A_1 - z)^{-j} - (A_0 - z)^{-j}\) of the form,

\[(2.15)\]

\[(A_1 - z)^{-j} - (A_0 - z)^{-j} = T_1^{(j)}(B) + \cdots + T_j^{(j)}(B, \ldots, B) + R_{j+1}^{(j)}(B; B, \ldots, B).\]

**Lemma 2.13.** Fix \(j = 1, \ldots, p\) and assume that \(B\) is a p-relative trace-class perturbation of \(A_0\). Set \(P_n = \chi_{[-n, n]}(A_0)\) and \(B_n := P_nBP_n\). The following assertions hold:

(i) For every \(i \in \mathbb{N}\) we have \(T_i^{(j)}(B, \ldots, B) \in \mathcal{L}_{\frac{i+1}{i+1}}(\mathcal{H})\).

(ii) For every \(i \in \mathbb{N}\) we have the convergence

\[
\lim_{n \to \infty} \left\| T_i^{(j)}(B_n, \ldots, B_n) - T_i^{(j)}(B, \ldots, B) \right\|_{\frac{i+1}{i+1}} = 0.
\]

(iii) For every \(i \in \mathbb{N}\) we have \(R_i^{(j)}(B; B, \ldots, B) \in \mathcal{L}_{\frac{i+1}{i+1}}(\mathcal{H})\).
(iv) For every $i \in \mathbb{N}$ we have the convergence
\[
\lim_{n \to \infty} \left\| R^{(j)}_i (B_n; B_n, \ldots, B_n) - R^{(j)}_i (B; B, \ldots, B) \right\|_{p+1} = 0.
\]

Proof. (i). Since the operator $B$ is a $p$-relative trace-class perturbation of $A_0$, Lemma 2.7 implies that
\[
(A_0 - z)^{-k_0-1} B(A_0 - z)^{-k_1-1} \in \mathcal{L}_{\frac{p+1}{k_0+k_1+2}}(\mathcal{H})
\]
and
\[
B(A_0 - z)^{-k_1-1} \in \mathcal{L}_{\frac{p+1}{k_1}}(\mathcal{H}), \quad l = 2, \ldots, i.
\]
Hence, by the Hölder inequality we have that
\[
(A_0 - z)^{-k_0-1} B(A_0 - z)^{-k_1-1} \cdots B(A_0 - z)^{-k_{j-1}-1} \in \mathcal{L}_{\frac{p+1}{k_0+k_1+\cdots+k_{j-1}}}(\mathcal{H}).
\]
Since $k_0 + k_1 + \cdots + k_{j-1} = j - 1$, we then obtain
\[
T^{(j)}_i (B, \ldots, B) = \sum_{k_0 + \cdots + k_{j-1} = j-1} (A_0 - z)^{-k_0-1} B(A_0 - z)^{-k_1-1} \cdots B(A_0 - z)^{-k_{j-1}-1}
\]
\[
\in \mathcal{L}_{\frac{p+1}{j-1}}(\mathcal{H}),
\]
as required.

(ii). Since $P_n \to 1$ in the strong operator topology, Lemma 2.7 and inclusions (2.16), (2.17) imply that
\[
(A_0 - z)^{-k_0-1} B_n(A_0 - z)^{-k_1-1} = P_n(A_0 - z)^{-k_0-1} B(A_0 - z)^{-k_1-1} P_n \
\rightarrow (A_0 - z)^{-k_0-1} B(A_0 - z)^{-k_1-1}
\]
in $\mathcal{L}_{\frac{p+1}{k_0+k_1+2}}(\mathcal{H})$ and
\[
B_n(A_0 - z)^{-k_l-1} = P_n B(A_0 - z)^{-k_l-1} P_n \to B(A_0 - z)^{-k_l-1}
\]
in $\mathcal{L}_{\frac{p+1}{k_l}}(\mathcal{H})$ for every $l = 2, \ldots, i$. Hence, using again the Hölder inequality, we conclude that
\[
\lim_{n \to \infty} \left\| T^{(j)}_i (B_n, \ldots, B_n) - T^{(j)}_i (B, \ldots, B) \right\|_{\frac{p+1}{j-1}} = 0.
\]

(iii). By Lemma 2.7 we have that
\[
B(A_0 - z)^{-1} \in \mathcal{L}_{p+1}(\mathcal{H}),
\]
which implies that
\[
B(A_0 - z)^{-k_l-1} \in \mathcal{L}_{p+1}(\mathcal{H}),
\]
for any $k_l \in \mathbb{Z}_+$. Therefore, by the Hölder inequality
\[
B(A_0 - z)^{-k_l-1} \cdots B(A_0 - z)^{-k_{j-1}-1} \in \mathcal{L}_{\frac{p+1}{k_0+k_1+\cdots+k_{j-1}}}(\mathcal{H}),
\]
that is
\[
R^{(j)}_i (B; B, \ldots, B) \in \mathcal{L}_{\frac{p+1}{j-1}}(\mathcal{H}).
\]
The proof of part (iv) can be obtained similarly to (ii) taking into account also that
\[
(A_0 + B_n - z)^{-l} \to (A_0 + B - z)^{-l}, \quad l \in \mathbb{N}
\]
in the strong operator topology (see Lemma 2.12 (i)).
The following theorem establishes, in particular, that the $p$-relative trace-class assumption implies that $A_1$ and $A_0$ are $p$-resolvent comparable and the difference $(A_0 + B - z)^{-p} - (A_0 - z)^{-p}$ can be approximated (in the trace-class norm) by $(A_0 + P_nBP_n - z)^{-p} - (A_0 - z)^{-p}$. The theorem is our first key result used in the proof of the principal trace formula. This result guarantees that Theorem 2.14 is applicable to the operators $A_0, A_0 + B$ and $A_0 + B_n$.

**Theorem 2.14.** Assume that $B$ is a $p$-relative trace-class perturbation of $A_0$. Set $P_n = \chi_{[-n,n]}(A_0)$ and $B_n := P_nBP_n$ and let $z \in \mathbb{C} \setminus \mathbb{R}$. For any $j = 1, \ldots, p$ we have that

$$(A_0 + B - z)^{-j} - (A_0 - z)^{-j} \in \mathcal{L}_{\frac{1}{j}}(\mathcal{H})$$

and $(A_0 + B_n - z)^{-j} - (A_0 - z)^{-j}$ converges to $(A_0 + B - z)^{-j} - (A_0 - z)^{-j}$ with respect to the norm of $\mathcal{L}_{\frac{1}{j}}(\mathcal{H})$. For any $j > p$ the assertion holds in the trace-class ideal $\mathcal{L}_1(\mathcal{H})$.

**Proof.** We prove the assertion for $j = 1, \ldots, p$ only, as the proof for $j > p$ is similar. Let $j = 1, \ldots, p$ be fixed. By (2.15) we can write

$$(A_0 + B - z)^{-j} - (A_0 - z)^{-j} = T^{(j)}(B) + \cdots + T^{(j)}(B, \ldots, B) + R^{(j)}_{j+1}(B; B, \ldots, B).$$

Hence, the first assertion follows from Lemma 2.13 (i) and (iii).

To prove convergence, we use (2.15) with $B_n$ instead of $B$ to write

$$\begin{align*}
(A_0 + B_n - z)^{-j} - (A_0 - z)^{-j} &= T^{(j)}(B_n) + \cdots + T^{(j)}(B_n, \ldots, B_n) + R^{(j)}_{j+1}(B_n; B_n, \ldots, B_n).
\end{align*}$$

Appealing to Lemma 2.13 (ii) and (iv) we conclude the proof. \hfill \Box

Next, we proceed with the discussion of the right-hand side of the principal trace formula (1.2). Let, as before, $B$ be a $p$-relative trace-class perturbation of a self-adjoint operator $A_0$. We introduce the straight-line path $\{A_s\}_{s \in [0,1]}$ joining $A_0$ and $A_0 + B$, by setting

$$A_s = A_0 + sB, \quad s \in [0,1].$$

We also introduce the path $\{A_{s,n}\}_{s \in [0,1]}$ joining $A_0$ and $A_0 + B_n$ by

$$A_{s,n} = A_0 + sB_n, \quad s \in [0,1], n \in \mathbb{N}.$$

We firstly note the following:

**Remark 2.15.** Repeating the proof of Theorem 2.14 replacing $B$ and $B_n$ by the operators $sB$ and $sB_n$, $s \in (0,1]$, respectively, one can conclude that the functions

$$s \mapsto \|(A_s - z)^{-j} - (A_0 - z)^{-j}\|_{\frac{1}{j+1}}$$

and

$$s \mapsto \|(A_{s,n} - z)^{-j} - (A_0 - z)^{-j}\|_{\frac{1}{j+1}}$$

are continuous with respect to $s$ and uniformly bounded with respect to $n \in \mathbb{N}$.

**Proposition 2.16.** Let $B$ be a $p$-relative trace-class perturbation of a self-adjoint operator $A_0$ and let $A_s = A_0 + sB, s \in [0,1]$. The function

$$s \mapsto e^{-tA_s^2}B, \quad t > 0,$$
is a continuous \( \mathcal{L}_1(\mathcal{H}) \)-valued function on \([0, 1]\). In particular, the integral

\[
\int_0^1 \text{tr} \left( e^{-tA_s^2} B \right) ds
\]

is well-defined.

**Proof.** Firstly we show that the operator \( e^{-tA_s^2} B \) is a trace class operator for any fixed \( s \in [0, 1] \). It is sufficient to show that the operator \( (A_s + i)^{-p-1} B \) is a trace-class operator. We may write

\[
(A_s + i)^{-p-1} B = (A_s + i)^{-p-1} - (A_0 + i)^{-p-1} + (A_0 + i)^{-p-1} B.
\]

As \( B \) is a \( p \)-relative trace-class perturbation of \( A_0 \) it follows that the second term on the right-hand side is a trace-class operator. For the first term, Theorem 2.14 implies the operator \( (A_s + i)^{-p-1} - (A_0 + i)^{-p-1} \) is a trace-class operator. Hence, \( (A_s + i)^{-p-1} B \in L_1(\mathcal{H}) \) for any \( s \in [0, 1] \), as required.

Now, we prove that the mapping \( s \mapsto e^{-tA_s^2} B \) is continuous in \( L_1(\mathcal{H}) \)-norm. Let \( s_1, s_2 \in [0, 1] \). We set

\[
p_0 = 2 \left\lfloor \frac{p}{2} \right\rfloor + 1.
\]

By Theorem 2.14 the operators \( A = A_{s_1} \) and \( B = A_{s_2} \) satisfy the assumption of Proposition 2.3. Therefore, we have

\[
e^{-tA_{s_1}^2} B - e^{-tA_{s_2}^2} B = \sum_{j=1,2} T_{f,a_j}^{A_{s_1},A_{s_2}} \left( (A_{s_1} - a_j i)^{-p_0} - (A_{s_2} - a_j i)^{-p_0} \right) \cdot B,
\]

where \( f(x) = e^{-tx^2}, x \in \mathbb{R}, t > 0 \).

By Remark 2.14 we have that

\[
\left\| (A_{s_1} - a_j i)^{-p_0} - (A_{s_2} - a_j i)^{-p_0} \right\|_1 \to 0, \quad \text{as } s_1 - s_2 \to 0.
\]

Furthermore, by Theorem 2.13 the double operator integral \( T_{f,a_j}^{A_{s_1},A_{s_2}} \), \( j = 1, 2 \), converges pointwise on \( L_1(\mathcal{H}) \) to \( T_{f,a_j}^{A_{s_1},A_{s_1}} \), as \( s_2 \to s_1 \). Therefore,

\[
\left\| T_{f,a_j}^{A_{s_1},A_{s_2}} \left( (A_{s_1} - a_j i)^{-p_0} - (A_{s_2} - a_j i)^{-p_0} \right) \right\|
\leq \left\| T_{f,a_j}^{A_{s_1},A_{s_2}} - T_{f,a_j}^{A_{s_1},A_{s_1}} \right\| \left( (A_{s_1} - a_j i)^{-p_0} - (A_{s_2} - a_j i)^{-p_0} \right)
+ \left\| T_{f,a_j}^{A_{s_1},A_{s_1}} \left( (A_{s_1} - a_j i)^{-p_0} - (A_{s_2} - a_j i)^{-p_0} \right) \right\|
\to 0, \quad s_1 - s_2 \to 0, \quad j = 1, 2.
\]

Thus, equality (2.21) implies that

\[
\left\| e^{-tA_{s_1}^2} B - e^{-tA_{s_2}^2} B \right\|_1 \to 0, \quad s_1 - s_2 \to 0,
\]

as required. \( \square \)

To conclude this section we prove that the integral in Proposition 2.16 can be approximated by a similar integral with \( B \) replaced by \( B_n \) (and so \( A_s \) replaced by \( A_{s,n} \)).
Proposition 2.17. We have that

\[(2.22) \quad \lim_{n \to \infty} \int_0^1 \text{tr} \left( e^{-tA_{s,n}^2} B_n \right) ds = \int_0^1 \text{tr} \left( e^{-tA_s^2} B \right) ds. \]

**Proof.** Let \( s \in [0, 1] \) be fixed. We write

\[ e^{-tA_{s,n}^2} B_n = (A_{s,n} + i)^{p+1} e^{-tA_{s,n}^2} \cdot (A_{s,n} + i)^{-p-1} B_n. \]

Since \( A_{s,n} \to A_s \) in the strong resolvent sense (see Lemma 2.12) and the function \( x \mapsto e^{-tx^2}(x + i)^{p+1}, x \in \mathbb{R} \), is continuous and bounded, [RS80] Theorem VIII.23 implies that \((A_{s,n} + i)^{p+1} e^{-tA_{s,n}^2} \to (A_s + i)^{p+1} e^{-tA_s^2}\) in the strong operator topology. Hence, by Lemma 2.9 to prove the convergence

\[(2.23) \quad \lim_{n \to \infty} \left\| e^{-tA_{s,n}^2} B_n - e^{-tA_s^2} B \right\|_1 = 0 \]

it is sufficient to show that

\[(2.24) \quad \lim_{n \to \infty} \left\| (A_{s,n} + i)^{-p-1} B_n - (A_s + i)^{-p-1} B \right\|_1 = 0. \]

To prove (2.24) we write

\[ (A_{s,n} + i)^{-p-1} B_n = \left( (A_{s,n} + i)^{-p-1} - (A_0 + i)^{-p-1} \right) B_n + P_n (A_0 + i)^{-p-1} BP_n \]

Theorem 2.14 implies that \( \left( (A_{s,n} + i)^{-p-1} - (A_0 + i)^{-p-1} \right) \) converges to \( (A_s + i)^{-p-1} - (A_0 + i)^{-p-1} \) in \( \mathcal{L}_1(\mathcal{H}) \). Moreover, combining the assumption that \((A_0 + i)^{-p-1} B \in \mathcal{L}_1(\mathcal{H})\) with the strong operator convergence \( P_n \to 1 \) and with Lemma 2.9 we obtain

\[ P_n (A_0 + i)^{-p-1} BP_n \to (A_0 + i)^{-p-1} B \]

in \( \mathcal{L}_1(\mathcal{H}) \). Hence, for every fixed \( s \in [0, 1] \), the sequence \( \{ (A_{s,n} + i)^{-p-1} B_n \}_{n \in \mathbb{N}} \) converges to \( (A_s + i)^{-p-1} B \) in \( \mathcal{L}_1(\mathcal{H}) \), which suffices to prove (2.23).

We claim that the sequence of functions

\[ s \mapsto \| e^{-tA_{s,n}^2} B_n \|_1, \quad s \in [0, 1], \quad t > 0, \]

is uniformly bounded (with respect to \( n \)) by a continuous function. Indeed, we have

\[ \| e^{-tA_{s,n}^2} B_n \|_1 \leq \| (A_{s,n} + i)^{p+1} e^{-tA_{s,n}^2} \| \cdot \| (A_{s,n} + i)^{-p-1} B_n \|_1 \]

\[ \leq \text{const} \| (A_{s,n} + i)^{-p-1} - (A_0 + i)^{-p-1} \| B_n \|_1 \]

\[ + \text{const} \| (A_0 + i)^{-p-1} B_n \|_1, \]

where the constant is independent of \( s \) and \( n \).

By Remark 2.13 the first term in the previous inequality involves a sequence of functions uniformly majorised by a continuous function. Since \( B_n = P_n BP_n \), the second term is clearly uniformly majorised by the constant function

\[ \text{const} \| (A_0 + i)^{-p-1} B \|_1. \]

Thus, appealing to (2.23) and the dominated convergence theorem we infer that

\[ \lim_{n \to \infty} \int_0^1 \text{tr} \left( e^{-tA_{s,n}^2} B_n \right) ds = \int_0^1 \text{tr} \left( e^{-tA_s^2} B \right) ds. \]

\[ \square \]
SPECTRAL FLOW AND INDEX

3. THE SETTING FOR OUR MAIN RESULT

In the present section we introduce the set-up for the rest of the paper as well as explain the approximation scheme we employ in our approach. The idea is to introduce a spectral ‘cut-off’ by the characteristic function of the interval \([-n, n]\) for positive integral \(n\). We use the subscript \(n\) on the operators introduced in the current section to indicate these spectrally cut-off or ‘reduced’ versions.

As we explained in the introduction we are interested in spectral flow, its relation to the Fredholm or Witten index and in its generalisation beyond the Fredholm setting, for certain paths of self-adjoint operators. We do not, in this article, aim for the maximum possible generality. There are more general formulations of our ideas but we confine the discussion to the completion of the program started in [GLM+11].

Following on from this motivating paper we now introduce precisely the operators we work with. Our paths are restricted by the final Hypothesis 5.1. In this introductory discussion however we will work under the less restrictive Hypothesis 3.1.

**Hypothesis 3.1.** Suppose \(\mathcal{H}\) is a complex, separable Hilbert space.

(i) Assume \(A_-\) is self-adjoint on \(\text{dom}(A_-) \subseteq \mathcal{H}\).

(ii) Suppose we have a family of bounded self-adjoint operators \(\{B(t)\}_{t \in \mathbb{R}} \subset \mathcal{B}(\mathcal{H})\), continuously differentiable with respect to \(t\) in the uniform operator norm, such that

\[
\|B'(\cdot)\| \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R}).
\]

(iii) Suppose that for some \(p \in \mathbb{N} \cup \{0\}\) we have

\[
B'(t)(A_- + i)^{-p-1} \in L^1(\mathcal{H}), \quad \int_{\mathbb{R}} \|B'(t)(A_- + i)^{-p-1}\|_1 \, dt < \infty.
\]

In what follows, we always choose the smallest \(p \in \mathbb{N} \cup \{0\}\) which satisfies (3.2).

Given Hypothesis 3.1 we introduce the family of self-adjoint operators \(A(t)\), \(t \in \mathbb{R}\), in \(\mathcal{H}\), by

\[
A(t) = A_- + B(t), \quad \text{dom}(A(t)) = \text{dom}(A_-), \quad t \in \mathbb{R}.
\]

Writing

\[
B(t) = B(t_0) + \int_{t_0}^{t} B'(s) \, ds, \quad t, t_0 \in \mathbb{R},
\]

with the convergent Bochner integral on the right-hand side, we conclude that the self-adjoint asymptotes

\[
\lim_{t \to \pm \infty} B(t) := B_{\pm} \in \mathcal{B}(\mathcal{H})
\]

exist. In particular, purely for convenience of notation, we will make the choice

\(B_- = 0\)

in the following and also introduce the asymptote,

\[
A_+ = A_- + B_+, \quad \text{dom}(A_+) = \text{dom}(A_-).
\]

Assumption 3.1 and equality (3.4) also yield,

\[
\sup_{t \in \mathbb{R}} \|B(t)\| \leq \int_{\mathbb{R}} \|B'(t)\| \, dt < \infty.
\]
A simple application of the resolvent identity yields (with \( t \in \mathbb{R}, z \in \mathbb{C} \setminus \mathbb{R} \))
\[
(A(t) - zI)^{-1} = (A_\pm - zI)^{-1} - (A(t) - zI)^{-1}B(t) - B_\pm|A_\pm - zI)^{-1},
\]
\[\| (A(t) - zI)^{-1} - (A_\pm - zI)^{-1} \| \leq |\text{Im}(z)|^{-2}\|B(t) - B_\pm\|,
\]
and hence proves that
\[
\text{n-lim}_{t \to \pm \infty} (A(t) - zI)^{-1} = (A_\pm - zI)^{-1}, \quad z \in \mathbb{C} \setminus \mathbb{R}.
\]
This is relevant to whether spectral flow between \( A_- \) and \( A_+ \) along the path \( \{A(t)\} \) exists.

Repeating the argument of [GLM+11 (3.49)] one can prove that
\[
(3.8) \quad B_+(A_- + i)^{-1-p}, \quad B(t)(A_- + i)^{-1-p} \in \mathcal{L}_1(\mathcal{H}),
\]
that is, \( B_+ \) as well as the family \( \{B(t)\}_{t \in \mathbb{R}} \) are \( p \)-relative trace-class perturbations with respect to \( A_- \). In particular, results of Section 2.2 apply to the perturbations \( B_+ \) and \( B(t), t \in \mathbb{R} \), of the operator \( A_- \).

As the next step in this section, we introduce the key technical ideas that enable us to use the old results of [GLM+11] in an approximation scheme.

As in Section 2.2 we introduce a spectral ‘cut-off’ of the operator \( A_- \) by setting
\[
P_n = \chi_{[-n,n]}(A_-). \quad \text{Recall also that } \text{s-lim}_{n \to \infty} P_n = 1.
\]

Let \( \{B(t)\}_{t \in \mathbb{R}} \) be a one parameter family of perturbations of \( A_- \) satisfying Hypothesis 4.2. We introduce the family \( \{B_n(t)\}_{t \in \mathbb{R}}, n \in \mathbb{N}, \) of reduced operators by setting
\[
(3.9) \quad B_n(t) := P_nB(t)P_n, \quad t \in \mathbb{R}, n \in \mathbb{N}.
\]
In this case,
\[
(3.10) \quad A_n(t) := A_- + B_n(t), \quad \text{dom}(A_n(t)) = \text{dom}(A_-), \quad n \in \mathbb{N}, t \in \mathbb{R}.
\]
In particular, one concludes that
\[
(3.11) \quad B_{+,n} := \text{n-lim}_{t \to +\infty} B_n(t) = P_nB_+P_n,
\]
and therefore for the reduced asymptotes \( A_{+,n} \), constructed with the family \( \{B(t)\}_{t \in \mathbb{R}} \) replaced by \( \{B_n(t)\}_{t \in \mathbb{R}} \), we obtain
\[
(3.12) \quad A_{+,n} := A_- + B_{+,n} = A_- + P_nB_+P_n, \quad \text{dom}(A_{+,n}) = \text{dom}(A_-).
\]
We note that the equality (3.8) together with the definition of the projections \( P_n \) implies that
\[
(3.13) \quad B_{+,n} = P_nB_+P_n \in \mathcal{L}_1(\mathcal{H}).
\]
The following proposition shows that the family \( \{B_n(t)\}_{t \in \mathbb{R}} \) of ‘approximants’ consists of trace-class operators, and so for this family the results of [Pus08] hold. The proof of this proposition is a verbatim repetition of the proof of [GLM+11 Proposition 2.3] and is therefore omitted.

**Proposition 3.2.** The family \( \{B_n(t)\}_{t \in \mathbb{R}} \) consists of trace-class perturbations of \( A_- \) and therefore satisfies the assumption in [Pus08] and [GLM+11].
Corresponding to the problem of studying spectral flow along a suitable path joining \( A_+ \) there is an index problem that we now introduce. Let \( A_- \) be the operator acting in \( L^2(\mathbb{R}; \mathcal{H}) \) defined by (1.5) with a constant fibre family \( \{ A_-(t) \}_{t \in \mathbb{R}} \), that is,

\[
(A_- f)(t) = A_- f(t),
\]

(3.14)

\[
f \in \text{dom}(A_-) = \left\{ g \in L^2(\mathbb{R}; \mathcal{H}) \mid g(t) \in \text{dom}(A_-) \text{ for a.e. } t \in \mathbb{R}; \int_{\mathbb{R}} \| A_- g(t) \|^2 dt < \infty \right\}.
\]

Identifying the Hilbert spaces \( L^2(\mathbb{R}; \mathcal{H}) \) and \( L^2(\mathbb{R}) \otimes \mathcal{H} \) we have that

\[
A_- = 1 \otimes A_-.
\]

Let the operators \( A, B, A' = B' \), be defined by (1.5) in terms of the families \( \{ A(t) \}_{t \in \mathbb{R}}, \{ B(t) \}_{t \in \mathbb{R}}, \text{ and } \{ B'(t) \}_{t \in \mathbb{R}} \), respectively. Since \( B(t), B'(t) \) are bounded operators for every \( t \in \mathbb{R} \) and \( \| B(\cdot) \|, \| B'(\cdot) \| \in L^\infty(\mathbb{R}) \) (see (3.7) and Hypothesis 3.1 (ii), respectively) we have that

\[
B, B' \in \mathcal{B}(L^2(\mathbb{R}; \mathcal{H})).
\]

Since, in addition, \( A(t) = A_- + B(t) \), we infer that

\[
A = A_- + B, \quad \text{dom}(A) = \text{dom}(A_-).
\]

Now, to introduce the operator \( D_A \) in \( L^2(\mathbb{R}; \mathcal{H}) \), we recall that the operator \( d/dt \) in \( L^2(\mathbb{R}; \mathcal{H}) \) is defined by

\[
\left( \frac{d}{dt} f \right)(t) = f'(t) \quad \text{for a.e. } t \in \mathbb{R},
\]

\[
f \in \text{dom}(d/dt) = \left\{ g \in L^2(\mathbb{R}; \mathcal{H}) \mid g \in AC_{\text{loc}}(\mathbb{R}; \mathcal{H}), g' \in L^2(\mathbb{R}; \mathcal{H}) \right\}
\]

(3.15)

\[
= W^{1,2}(\mathbb{R}; \mathcal{H}).
\]

Then, the operator \( D_A \) is defined by setting

\[
D_A = \frac{d}{dt} + A, \quad \text{dom}(D_A) = W^{1,2}(\mathbb{R}; \mathcal{H}) \cap \text{dom}(A_-).
\]

Assuming Hypothesis 3.1 and repeating the proof of (GLM+11) Lemma 4.4] one can show that the operator \( D_A \) is densely defined and closed in \( L^2(\mathbb{R}; \mathcal{H}) \). Furthermore, the adjoint operator \( D_A^* \) of \( D_A \) in \( L^2(\mathbb{R}; \mathcal{H}) \) is then given by (cf. (GLM+11))

\[
D_A^* = -\frac{d}{dt} + A, \quad \text{dom}(D_A^*) = W^{1,2}(\mathbb{R}; \mathcal{H}) \cap \text{dom}(A_-).
\]

This enables us to introduce the non-negative, self-adjoint operators \( H_j, j = 1, 2, \) in \( L^2(\mathbb{R}; \mathcal{H}) \) by

\[
H_1 = D_A^* D_A, \quad H_2 = D_A D_A^*.
\]

The following result is proved in [CGP+17 Theorem 2.6] under a relatively trace class perturbation assumption. It was already noted in [CGP+17 Remark 2.7] that the result holds without this assumption. Thus, in our more general setting the following theorem holds.
Theorem 3.3. Assume Hypothesis 3.1. Then the operator $D_A$ is Fredholm if and only if $0 \in \rho(A_+) \cap \rho(A_-)$.

Next, we turn to the reduced counterparts $H_{j,n}, j = 1, 2, n \in \mathbb{N}$, of the operators $H_j, j = 1, 2$. Recall that the family $\{B_n(t)\}_{t \in \mathbb{R}}$, $n \in \mathbb{N}$ is defined by (see (3.11))

$$B_n(t) = P_n B(t) P_n, \quad P_n = \chi_{[-n,n]}(A_-).$$

In this case, the corresponding operator $A_n$ is defined as

$$A_n = A_- + B_n,$$

where $B_n$ is defined by (1.5) with $\{T(t)\}_{t \in \mathbb{R}} = \{B_n(t)\}_{t \in \mathbb{R}}$.

Denote by $H_{j,n}, j = 1, 2$, the operator defined by (3.17) with $D_A$ replaced by the corresponding operator $D_{A_n} = \frac{d}{dt} + A_n$.

4. SOME UNIFORM NORM ESTIMATES

In this section we prove some uniform norm estimates for the operators $H_j, j = 1, 2$. This result will be used in the proof of the second key result of this Section, Theorem 5.2. The methods are borrowed from the abstract pseudo-differential calculus of non-commutative geometry [CGRS14, CGP+15, CM95].

For future purposes we also introduce $H_0$ in $L^2(\mathbb{R}; \mathcal{H})$ by

$$(4.1) \quad H_0 = -\frac{d^2}{dt^2} + A^2, \quad \text{dom}(H_0) = W^{2,2}(\mathbb{R}; \mathcal{H}) \cap \text{dom}(A_+^2).$$

By [RS80, Theorem VIII.33], the operator $H_0$ is self-adjoint and positive. We note that the operators $A_- \text{ and } H_0$ commute and

$$(4.2) \quad \text{dom} H_0^{1/2} = \text{dom}(d/dt) \cap \text{dom} A_-.$$  

The proof of the following result can be found in [GLM+11, Lemma 4.7]. Observe, that the proof given there does not require the full strength of the assumptions made in that paper. The statement is formulated using Hypothesis 3.1. In fact, it requires only Hypothesis 3.1 (i).

Lemma 4.1. [GLM+11, Lemma 4.7] For every $z < 0$, the operator $A_- (H_0 - z)^{-1/2}$ is bounded and

$$\|A_- (H_0 - z)^{-1/2}\| \leq 1, \quad z < 0.$$  

In the context of Lemma 4.1, we note also that

$$(4.3) \quad \frac{d}{dt} \cdot (H_0 + 1)^{-1/2} \in \mathcal{B}(L^2(\mathbb{R}; \mathcal{H})).$$

In what follows, we need to strengthen Hypothesis 3.1 as follows.

Hypothesis 4.2. In addition to Hypothesis 3.1, assume that $\text{dom}(H_0^{1/2})$ is invariant with respect to the operator $B$.

Assuming Hypothesis 4.2 in the following, we have that $A_- B$ is an operator well defined on $\text{dom} H_0^{1/2}$, since $\text{dom} H_0^{1/2} \subset \text{dom} A_-$ (see (4.2)). Therefore, recalling that $A = A_- + B$ one can decompose $H_j, j = 1, 2$, as follows

$$H_j = -\frac{d^2}{dt^2} + A^2 + (-1)^j A'$$

$$(4.4) \quad = H_0 + B A_- + A_- B + B^2 + (-1)^j B', \quad \text{dom}(H_j) = \text{dom}(H_0), \quad j = 1, 2.$$
For convenience, we set

\[(H_j - zI)^{-1} - (H_0 - zI)^{-1} = -(H_j - zI)^{-1}(H_j - H_0)(H_0 - zI)^{-1}\]

(4.5)

for \(j = 1, 2\) and \(z \in \mathbb{C} \setminus \mathbb{R}_+\).

Assuming Hypothesis 4.2, one obtains, similarly to the proof of (4.4), the decompositions for the operators \(H_{j,n}, j = 1, 2\), of the following form

\[H_{j,n} = \frac{d^2}{dt^2} + A_n^2 + (-1)^j A_n^j\]

(4.6)

where \(P_n = \chi_{[-n,n]}(A_{-}) = 1 \otimes P_n\).

The following result can be found in [CGLS16a, Lemma 3.12 (i)].

**Lemma 4.3.** Assume Hypothesis 4.2. The operators \(H_{j,n}\) converge to \(H_j\), \(j = 1, 2\), in the strong resolvent sense.

For \(k \in \mathbb{N}\) we introduce

\[\operatorname{dom}(\delta^k_{H_0}) = \{T \in \mathcal{B}(L^2(\mathbb{R}; \mathcal{H})) : T \operatorname{dom}(H_0^{j/2}) \subset \operatorname{dom}(H_0^{j/2}), \forall j = 1, \ldots, k,\]

and the operator \([[(1 + H_0)^{1/2}, T]]^{(k)}\), defined on \(\operatorname{dom}(H_0^{k/2})\),

extends to a bounded operator on \(L^2(\mathbb{R}; \mathcal{H})\).

and set

\[\delta^k_{H_0}(T) = [[[1 + H_0]^{1/2}, T]^{(k)}], \quad T \in \operatorname{dom}(\delta^k_{H_0}).\]

(4.7)

where the notation \([[[1 + H_0]^{1/2}, T]]^{(k)}\) stands for \(k\)-th repeated commutator defined by

\[\{[(1 + H_0)^{1/2}, T]]^{(k)} = [(1 + H_0)^{1/2}, \ldots, [(1 + H_0)^{1/2}, [(1 + H_0)^{1/2}, T]] \ldots,\]

\[\operatorname{dom}([[1 + H_0]^{1/2}, T]]^{(k)}) = \operatorname{dom}(H_0^{k/2}).\]

For convenience, we set

\[[[1 + H_0]^{1/2}, T]]^{(0)} = T.\]

**Remark 4.4.** Note that \(\bigcap_{j=0}^k \operatorname{dom}(\delta^j_{H_0})\), \(k \in \mathbb{N}\), is a subalgebra in \(\mathcal{B}(L^2(\mathbb{R}; \mathcal{H}))\).

We note that if \(T \in \operatorname{dom}(\delta_{H_0})\), then for every \(\xi \in \operatorname{dom}(H_0^{1/2})\) we have

\[T(H_0 + 1)^{1/2}\xi = (H_0 + 1)^{1/2} T\xi - [[(H_0 + 1)^{1/2}, T] T\xi.\]
Hence, if $T \in \bigcap_{j=1}^k \text{dom}(\delta_{H_j})$, for some $k \in \mathbb{N}$, then for every $\xi \in \text{dom}(H_0^{1/2})$, using this equality repeatedly, we obtain
\[
T(H_0 + 1)^{k/2} \xi = T(H_0 + 1)^{1/2} (H_0 + 1)^{k/2-1} \xi \\
= (H_0 + 1)^{1/2} T(H_0 + 1)^{k-1/2} \xi - [(H_0 + 1)^{1/2}, T](H_0 + 1)^{k-1/2} \xi \\
= \ldots \\
= \sum_{j=0}^k (-1)^j C_k^j (H_0 + 1)^{1/2} [(H_0 + 1)^{1/2}, T]^{k-j} \xi,
\]
where $C_k^j$ denotes the binomial coefficient.

**Lemma 4.5.** Assume $B \in \text{dom}(\delta_{H_0})$. Then the operator $(H_i + 1)^{-1/2}(H_0 + 1)^{1/2}, i = 1, 2$, defined on $\text{dom}(H_0^{1/2})$ extends to a bounded operator on $L^2(\mathbb{R}; \mathcal{H})$ and
\[
\left\| (H_i + 1)^{-1/2}(H_0 + 1)^{1/2} \right\| \leq \text{const} \cdot (\| \delta_{H_0}(B) \| + \| B \| + \| B' \| + \| B' \|). \]

**Remark 4.6.** Note that the first assertion in Lemma 4.5 follows immediately from the closed graph theorem and the fact that $\text{dom}(H_0) = \text{dom}(H_i), i = 1, 2$. However, we also need an estimate on the uniform norm of this operator.

**Proof.** Since the operator $H_1$ is self-adjoint and positive we can write
\[
(H_1 + 1)^{-1/2} = \frac{1}{\pi} \int_0^\infty \frac{d\lambda}{\lambda^{1/2}} (1 + \lambda + H_1)^{-1},
\]
with the right-hand side being a convergent Bochner integral (see e.g. [Kat95, p. 282]).

By the resolvent identity (4.5) for all $\xi \in \text{dom}(H_0)^{1/2}$ we have
\[
(H_i + 1)^{-1/2}(H_0 + 1)^{1/2} \xi \\
= \xi + \frac{1}{\pi} \int_0^\infty \frac{d\lambda}{\lambda^{1/2}} (1 + \lambda + H_1)^{-1} A_+ B(H_0 + 1)^{1/2} (1 + \lambda + H_0)^{-1} \xi \\
+ \frac{1}{\pi} \int_0^\infty \frac{d\lambda}{\lambda^{1/2}} (1 + \lambda + H_1)^{-1} B A_-(H_0 + 1)^{1/2} (1 + \lambda + H_0)^{-1} \xi \\
+ \frac{1}{\pi} \int_0^\infty \frac{d\lambda}{\lambda^{1/2}} (1 + \lambda + H_1)^{-1} (B^2 - B')(H_0 + 1)^{1/2} (1 + \lambda + H_0)^{-1} \xi
\]
(4.9)
\[
= \xi + I_1 \xi + I_2 \xi + I_3 \xi.
\]

The estimates
\[
\left\| (H_0 + 1)^{1/2} (1 + \lambda + H_0)^{-1} \right\| \leq (1 + \lambda)^{-1/2}, \quad \left\| (1 + \lambda + H_1)^{-1} \right\| \leq (1 + \lambda)^{-1},
\]
the fact that the operators $B, B'$ are bounded imply that the integral $I_3$ on the right-hand side of (4.9) converges in the uniform norm and
\[
\| I_3 \| \leq \text{const} (\| B \| + \| B' \|).
\]

Similarly for $I_2$, using in addition Lemma 4.1 we have
\[
\left\| A_- (H_0 + 1)^{1/2} (1 + \lambda + H_0)^{-1} \right\| \leq (1 + \lambda)^{-1/2},
\]
guaranteeing that the integral $I_2$ converges in the operator norm and
\[
\| I_2 \| \leq \text{const} \cdot \| B \|.
\]
Finally, for the integral $I_1$ we write

$$I_1 = \frac{1}{\pi} \int_0^\infty \frac{d\lambda}{\lambda^{1/2}}(1 + \lambda + H_1)^{-1} A_+ B (H_0 + 1)^{1/2} (1 + \lambda + H_0)^{-1} \xi$$

$$= \frac{1}{\pi} \int_0^\infty \frac{d\lambda}{\lambda^{1/2}}(1 + \lambda + H_1)^{-1} A_+ (H_0 + 1)^{-1/2} B (H_0 + 1)(1 + \lambda + H_0)^{-1} \xi$$

$$+ \frac{1}{\pi} \int_0^\infty \frac{d\lambda}{\lambda^{1/2}}(1 + \lambda + H_1)^{-1} A_-(H_0 + 1)^{-1/2}$$

$$\cdot [(H_0 + 1)^{1/2}, B] (H_0 + 1)^{1/2}(1 + \lambda + H_0)^{-1} \xi.$$

Since, $B \in \text{dom}(\delta_{H_0})$, the operator $[(H_0 + 1)^{1/2}, B]$ extends to a bounded operator on $L^2(\mathbb{R}; \mathcal{H})$. Hence, repeating the argument above, we conclude that $I_1$ is a bounded operator with

$$\|I_1\| \leq \text{const} \cdot (\|B\| + \|\delta_{H_0}(B)\|).$$

Thus, by (4.9) we have that the operator $(H_0 + 1)^{-1/2}(H_1 + 1)^{1/2}$ extends to a bounded operator on $L^2(\mathbb{R}; \mathcal{H})$ and

$$\left\|(H_0 + 1)^{-1/2}(H_1 + 1)^{1/2}\right\| \leq \text{const}(1 + \|\delta_{H_0}(B)\| + \|B\| + \|B\|^2 + \|B'\|).$$

The following result will be used later in the proof of the convergence of the left-hand side of the principal trace formula.

**Proposition 4.7.** Assume $B, B' \in \bigcap_{j=1}^{k-1} \text{dom}(\delta_{H_0}^j)$ for some $k \geq 2$. Then the operator $(H_i + 1)^{-k/2}(H_0 + 1)^{k/2}, i = 1, 2$, defined on $\text{dom}(H_0^{k/2})$ extends to a bounded operator on $L^2(\mathbb{R}; \mathcal{H})$ and

$$\left\|(H_i + 1)^{-k/2}(H_0 + 1)^{k/2}\right\| \leq \text{const} \cdot Q(\|\delta_{H_0}^j(B)\|, \|\delta_{H_0}^j(B')\|),$$

for all $j = 0, \ldots, k - 1$ and for some polynomial $Q$ with positive coefficients.

**Proof.** We prove the assertion only for $i = 1$, since the proof for $i = 2$ is identical.

We proceed by induction on $k$. For $k = 1$ the assertion is proved in Lemma 4.5.

Let $k = 2$. By the resolvent identity (4.5) we have

$$(H_1 + 1)^{-1}(H_0 + 1)\xi$$

$$= \xi - (H_1 + 1)^{-1} BA_- \xi - (H_1 + 1)^{-1} A_- B \xi$$

$$- (H_1 + 1)^{-1}(B^2 - B')\xi$$

for all $\xi \in \text{dom}(H_0)$. For the second term, using the fact that $A$ and $H_0$ commute, we write

$$(H_1 + 1)^{-1} BA_- \xi = (H_1 + 1)^{-1} B (H_0 + 1)^{1/2} A_- (H_0 + 1)^{-1/2} \xi$$

$$= (H_1 + 1)^{-1/2} \cdot (H_1 + 1)^{-1/2} (H_0 + 1)^{1/2} \cdot BA_- (H_0 + 1)^{-1/2} \xi$$

$$- (H_1 + 1)^{-1} [(H_0 + 1)^{1/2}, B] A_- (H_0 + 1)^{-1/2} \xi.$$

By Lemma 4.5, the operator $(H_1 + 1)^{-1/2}(H_0 + 1)^{1/2}$ extends to a bounded operator, and by the assumption $[(H_0 + 1)^{1/2}, B]$ also extends to a bounded operator.
Hence, the operator $(H_1 + 1)^{-1}BA_-$ extends to a bounded operator and
\[
\|(H_1 + 1)^{-1}BA_-\| \leq \|(H_1 + 1)^{1/2}(H_0 + 1)^{-1/2}\|\|B\| + \|\delta_{H_0}(B)\|
\leq \text{const} \cdot (1 + \|\delta_{H_0}(B)\| + \|B\| + \|B\|^2 + \|B'\|\|B\|)
\]
where the latter inequality follows from Lemma 4.5.

For the third term on the right hand side (4.10), we write
\[
(H_1 + 1)^{-1}A_\cdot B \xi = (H_1 + 1)^{-1/2} \cdot (H_1 + 1)^{-1/2}(H_0 + 1)^{1/2}
\times (H_0 + 1)^{-1/2}A_\cdot B \xi,
\]
for $\xi \in \text{dom}(H_0)$, and therefore, by Lemma 4.3 we conclude that $(H_1 + 1)^{-1}A_\cdot B$
onlyear{5} also extends to a bounded operator.

Thus, $(H_1 + 1)^{-1}(H_0 + 1)$ extends to a bounded operator and by (4.10) we have
\[
\|(H_1 + 1)^{-1}(H_0 + 1)\| \leq 1 + \|(H_1 + 1)^{-1}BA_-\|
+ \|(H_1 + 1)^{-1}A_\cdot B\| + \|(H_1 + 1)^{-1}(B^2 - B')\|
\leq Q(\|\delta_{H_0}(B)\|), \quad j = 0, 1.
\]
for some polynomial $Q$.

Suppose now that for some $k \geq 3$ the assertion holds for all $j \leq k - 1$. Let us prove it for $j = k$. For $\xi \in \text{dom}(H_0^{k/2})$, using the resolvent identity (4.3) we write
\[
(H_1 + 1)^{-k/2}(H_0 + 1)^{k/2}\xi = (H_1 + 1)^{-(k-2)/2}(H_1 + 1)^{-1}(H_0 + 1)^{k/2}\xi
\]
\[
= (H_1 + 1)^{-(k-2)/2}(H_0 + 1)^{(k-2)/2}\xi
\]
\[
+ (H_1 + 1)^{-k/2}(BA_- + A_\cdot B + B^2 - B')(H_0 + 1)^{(k-2)/2}\xi.
\]
By the induction hypothesis, the operator $(H_1 + 1)^{-(k-2)/2}(H_0 + 1)^{(k-2)/2}$ extends to a bounded operator with the required estimate in the uniform norm.

For the second term on the right hand side of (4.11) equality (4.3) implies that
\[
\sum_{j=0}^{k-1}(-1)^j C_k^j (H_1 + 1)^{-k/2}(H_0 + 1)^{j/2}[(H_0 + 1)^{1/2}, B^{(j)}]A_-(H_0 + 1)^{-1/2}\xi
\]
\[
+ \sum_{j=0}^{k-2}(-1)^j C_k^j (H_1 + 1)^{-k/2}(H_0 + 1)^{(j+1)/2}A_-(H_0 + 1)^{-1/2}[(H_0 + 1)^{1/2}, B^{(j)}]\xi
\]
\[
+ \sum_{j=0}^{k-2}(-1)^j C_k^j (H_1 + 1)^{-k/2}(H_0 + 1)^{j/2}[(H_0 + 1)^{1/2}, B^2 - B']^{(j)}\xi
\]
By the induction hypothesis, for every $j = 0, \ldots, k - 1$, it follows that the operator
\[
(H_1 + 1)^{-k/2}(H_0 + 1)^{j/2}
\]
extends to a bounded operator. In addition, the operators
\[
[(H_0 + 1)^{1/2}, B^{(j)}] \text{ and } [(H_0 + 1)^{1/2}, B']^{(j)}
\]
also extend to bounded operators by the assumption of the proposition. Hence,
\[(H_1 + 1)^{-k/2}(BA_+ + A_-B + B^2 - B')(H_0 + 1)^{(k-2)/2}\]
extends to a bounded operator and the required estimate in the uniform norm follows. □

**Proposition 4.8.** Let $B, B' \in \bigcap_{j=1}^{k-1} \text{dom}(\delta_{H_j}^j)$ for some $k \in \mathbb{N}$ and let $z \in \mathbb{C} \setminus \mathbb{R}$. Then

(i) The operator $(H_0 - z)^{k/2}(H_i - z)^{-k/2}$, $i = 1, 2$, is bounded.

(ii) The operators $(H_{i,n} - z)^{-k/2}(H_0 - z)^{k/2}$, and $(H_0 - z)^{k/2}(H_{i,n} - z)^{-k/2}$, $i = 1, 2$, are bounded.

(iii) The sequences
\[
\left\{ (H_{i,n} - z)^{-k/2}(H_0 - z)^{k/2} \right\}_{n=1}^\infty, \quad \left\{ (H_0 - z)^{k/2}(H_{i,n} - z)^{-k/2} \right\}_{n=1}^\infty
\]
are uniformly bounded.

**Proof.** Without loss of generality we can assume that $z = -1$.

(i). As the operators $(H_0 + 1)^{k/2}$ and $(H_{i,n} + 1)^{-k/2}$ are self-adjoint, both of the operators $(H_{i,n} + 1)^{-k/2}$ and $(H_{i,n} + 1)^{-k/2}(H_0 + 1)^{k/2}$ are densely defined, [Wei80] Theorem 4.19 (b) implies that
\[
(H_0 + 1)^{k/2}(H_i + 1)^{-k/2} = \left( (H_i + 1)^{-k/2}(H_0 + 1)^{k/2} \right)^* = \left( (H_i + 1)^{-k/2}(H_0 + 1)^{k/2} \right)^* \in \mathcal{B}(L^2(\mathbb{R};\mathcal{H})),
\]
where the last inclusion follows from Proposition 4.7.

(ii). Since $B, B' \in \bigcap_{j=1}^{k-1} \text{dom}(\delta_{H_j}^j)$, $B_n = P_nBP_n$, $B'_n = P_nB'P_n$, and $P_n$ commutes with $H_0$, we infer that $B_n, B'_n \in \bigcap_{j=1}^{k-1} \text{dom}(\delta_{H_j}^j)$. Therefore, applying Proposition 4.7 and part (i) to the operators $H_{i,n}$ and $H_0$, we obtain the assertion.

(iii). Note that for $j = 1, \ldots, k-1$, we have
\[
\|\delta_{H_0}^j(B_n)\| \leq \|\delta_{H_0}^j(B)\|, \quad \|\delta_{H_0}^j(B_n')\| \leq \|\delta_{H_0}^j(B')\|.
\]
Hence, Proposition 4.7 applied to the operators $H_{i,n}$ and $H_0$ implies that for some polynomial $Q$ with positive coefficients, we have
\[
\left\| (H_{i,n} + 1)^{-k/2}(H_0 + 1)^{k/2} \right\| \leq \text{const} Q(\|\delta_{H_0}^j(B_n)\|, \|\delta_{H_0}^j(B_n')\|)
\]
\[
\leq \text{const} Q(\|\delta_{H_0}^j(B)\|, \|\delta_{H_0}^j(B')\|), \quad j = 0, \ldots, k-1,
\]
which together with the equality
\[
\left\| (H_0 - z)^{k/2}(H_{i,n} - z)^{-k/2} \right\| = \left\| (H_{i,n} + 1)^{-k/2}(H_0 + 1)^{k/2} \right\|
\]
concludes the proof. □

**Corollary 4.9.** Let $B, B' \in \bigcap_{j=1}^{k-1} \text{dom}(\delta_{H_j}^j)$ for some $k \in \mathbb{N}$. Then
\[
\text{dom}(H_{i,n}^{k/2}) = \text{dom}(H_i^{k/2}) \subset \text{dom}(H_0^{k/2}), \quad i = 1, 2, \quad n \in \mathbb{N}.
\]

**Proof.** We prove only the equality $\text{dom}(H_0^{k/2}) = \text{dom}(H_1^{k/2})$ since the others can be proved similarly.
Let $\xi \in \text{dom}(H^{k/2}) = \text{dom}(H_1 + 1)^{k/2} = \text{ran}((H_1 + 1)^{-k/2})$. Then there exists $\eta \in L^2(\mathbb{R}; \mathcal{H})$ such that $\xi = (H_1 + 1)^{-k/2}\eta$. Since $\eta \in L^2(\mathbb{R}; \mathcal{H})$ and by Corollary 4.8 (i) the operator $(H_0 + 1)^{k/2}(H_1 + 1)^{-k/2}$ is bounded, we have that

$$(H_0 + 1)^{k/2} \xi = (H_0 + 1)^{k/2}(H_1 + 1)^{-k/2} \eta \in \mathcal{H},$$

that is $\xi \in \text{dom}(H_0 + 1)^{k/2} = \text{dom}(H_0^{k/2})$. \hfill \Box

By Propositions 4.7 and 4.8, the operators $(H_{2,n} - z)^{-\frac{k}{2}}(H_0 - z)^{-\frac{k}{2}}, \ n \in \mathbb{N},$ and $(H_2 - z)^{-\frac{k}{2}}(H_0 - z)^{-\frac{k}{2}}$ are bounded for every $z \in \mathbb{C} \setminus \mathbb{R}$. The following proposition establishes the strong-operator convergence of the sequences $\{(H_{2,n} - z)^{-\frac{k}{2}}(H_0 - z)^{-\frac{k}{2}}\}_{n \in \mathbb{N}}$ to $(H_2 - z)^{-\frac{k}{2}}(H_0 - z)^{-\frac{k}{2}}$, which is required for the proof of the principal trace formula. The result here should be compared with [CGLS16a, Lemma 3.13 (ii)], where a much simpler case $k = 2$ was treated.

**Proposition 4.10.** Assume that $B, B' \in \bigcap_{j=1}^{k-1} \text{dom}(\hat{\sigma}_H^j)$ for some $k \in \mathbb{N}$ and let $z \in \mathbb{C} \setminus \mathbb{R}$. Then

(i) $(H_{2,n} - z)^{-\frac{k}{2}}(H_0 - z)^{-\frac{k}{2}}$ converges to $(H_2 - z)^{-\frac{k}{2}}(H_0 - z)^{-\frac{k}{2}}$ in the strong operator topology.

(ii) $(H_2 - z)^{-\frac{k}{2}}(H_1,n - z)^{-\frac{k}{2}}$ converges to $(H_2 - z)^{-\frac{k}{2}}(H_1 - z)^{-\frac{k}{2}}$ in the strong operator topology.

**Proof.** Without loss of generality we have $z = -1$.

(i). By Lemma 4.9 we have that $H_{2,n} \to H_2$ in the strong resolvent sense. Therefore, [RS80, Theorem VIII.20] implies that $(H_{2,n} + 1)^{-\frac{k}{2}} \to (H_2 + 1)^{-\frac{k}{2}}$ in the strong operator topology. Hence, for every $\xi \in \text{dom}(H_2^{\frac{k}{2}})$ we have

$$(H_{2,n} + 1)^{-\frac{k}{2}}(H_0 + 1)^{-\frac{k}{2}} \xi \to (H_2 + 1)^{-\frac{k}{2}}(H_0 + 1)^{-\frac{k}{2}} \xi.$$

Since $\text{dom}(H_0^{\frac{k}{2}})$ is a dense subset in $L^2(\mathbb{R}; \mathcal{H})$ and by Proposition 4.8 (iii) the sequence $\{(H_{2,n} + 1)^{-\frac{k}{2}}(H_0 + 1)^{-\frac{k}{2}}\}_{n \in \mathbb{N}}$ is uniformly bounded, we infer that

$$(H_{2,n} + 1)^{-\frac{k}{2}}(H_0 + 1)^{-\frac{k}{2}} \to (H_2 + 1)^{-\frac{k}{2}}(H_0 + 1)^{-\frac{k}{2}}$$

in the strong operator topology.

(ii). By Corollary 4.9 we have that

$$\text{dom}(H_1 + 1)^{\frac{k}{2}} = \text{dom}(H_{1,n} + 1)^{\frac{k}{2}} \subset \text{dom}(H_0 + 1)^{\frac{k}{2}},$$

and therefore both $(H_{1,n} + 1)^{-\frac{k}{2}} \xi$ and $(H_1 + 1)^{-\frac{k}{2}} \xi$ lie in $\text{dom}(H_0 + 1)^{\frac{k}{2}}$ for every $\xi \in L^2(\mathbb{R}; \mathcal{H})$. The strong resolvent convergence $H_{1,n} \to H_1$ and [RS80, Theorem VIII.20], imply that $(H_{1,n} + 1)^{-\frac{k}{2}} \to (H_1 + 1)^{-\frac{k}{2}}$ in the strong operator topology. Hence, $(H_0 + 1)^{\frac{k}{2}}(H_{1,n} + 1)^{-\frac{k}{2}} \xi \to (H_0 + 1)^{\frac{k}{2}}(H_1 + 1)^{-\frac{k}{2}} \xi$ for every $\xi \in L^2(\mathbb{R}; \mathcal{H})$, since the operator $(H_0 + 1)^{\frac{k}{2}}$ is closed. \hfill \Box
5. The main hypothesis and the approximation result for the pair 
\((H_2, H_1)\)

In this section we give the precise hypotheses that we impose for our results and expand on the details of what they mean. Furthermore, we develop further our approximation scheme that is essential for the proof of the principal trace formula in Section 4 below.

**Hypothesis 5.1.**

(i) Assume \(A_\pm\) is self-adjoint on \(\text{dom}(A_\pm) \subseteq \mathcal{H}\) with \(\mathcal{H}\) a complex, separable Hilbert space.

(ii) Suppose we have a family of bounded self-adjoint operators \(\{B(t)\}_{t \in \mathbb{R}} \subseteq \mathcal{B}(\mathcal{H})\), continuously differentiable with respect to \(t\) in the uniform operator norm, such that \(\|B'(t)\| \in L^1(\mathbb{R}; dt) \cap L^\infty(\mathbb{R}; dt)\).

(iii) Suppose that for some \(p \in \mathbb{N} \cup \{0\}\), we have

\[
B'(t)(A_\pm + i)^{-p-1} \in \mathcal{L}_1(\mathcal{H}), \quad \int_{\mathbb{R}} \|B'(t)(A_\pm + i)^{-p-1}\|_1 dt < \infty.
\]

(iv) Let \(m = \left\lfloor \frac{p}{2} \right\rfloor\). Assume that for all \(z < 0\) we have that

\[
B'(H_0 - z)^{-m-1} \in L^1(\mathbb{R}; H_0).
\]

(v) \(B, B' \in \bigcap_{j=1}^{2m-1} \text{dom}(\delta_{H_0})\), where \(\delta_{H_0}\) is defined in (4.7).

In what follows we always take the smallest \(p \in \mathbb{N} \cup \{0\}\) satisfying (iii).

Assuming now Hypothesis 5.1 we can prove our second key result, which guarantees that we can use approximation on the left-hand side of the principal trace formula. The proof of this result crucially uses the results obtained in Section 4.

**Theorem 5.2.** Assume Hypothesis 5.1. Let \(z \in \mathbb{C} \setminus \mathbb{R}_+\).

(i) Both \((H_2 - z)^{-m} - (H_1 - z)^{-m}\) and \((H_{2,n} - z)^{-m} - (H_{1,n} - z)^{-m}\) are trace class.

(ii) We have

\[
\lim_{n \to \infty} \left\| (H_{2,n} - z)^{-m} - (H_{1,n} - z)^{-m} \right\|_1 = 0.
\]

**Proof.** (i). Using again the resolvent identity and the elementary relation

\[
A^k - B^k = \sum_{j=1}^{k} A^{k-j} [A - B] B^{j-1}, \quad A, B \in \mathcal{B}(\mathcal{H}), \; k \in \mathbb{N},
\]

we write

\[
(H_2 - z)^{-m} - (H_1 - z)^{-m}
\]

\[
= \sum_{j=1}^{m} (H_2 - z)^{-m+j} ((H_2 - z)^{-1} - (H_1 - z)^{-1}) (H_1 - z)^{-j+1}
\]

\[
= -2 \sum_{j=1}^{m} (H_2 - z)^{-m+j-1} B'(H_1 - z)^{-j}.
\]

Thus

\[
(H_2 - z)^{-m} - (H_1 - z)^{-m} = -2 \sum_{j=1}^{m} (H_2 - z)^{-m+j-1} (H_0 - z)^{m-j+1}
\]

\[
\times (H_0 - z)^{-m+j-1} B'(H_0 - z)^{-j} \times (H_0 - z)^{j} (H_1 - z)^{-j}
\]

(5.1)
We note that by the three lines theorem (see also [GLST15, Theorem 3.2]), Hypothesis 5.1 (iv) implies that

\[(H_0 - z)^{-m+j-1} B'(H_0 - z)^{-j} \in L_1(L^2(\mathbb{R}; \mathcal{H}))\]

for all \(j = 1, \ldots, m\). Since, in addition, by Proposition 4.8 (i) and (ii), the operators \((H_2 - z)^{-m+j-1}(H_0 - z)^{m-j+1}\) and \((H_0 - z)^j(H_1 - z)^{-j}\) are bounded, we infer that \((H_2 - z)^{-m} - (H_1 - z)^{-m} \in L_1(L^2(\mathbb{R}; \mathcal{H}))\).

Arguing similarly, one may obtain that

\[(H_{2,n} - z)^{-m} - (H_{1,n} - z)^{-m} = -2 \sum_{j=1}^{m} (H_{2,n} - z)^{-m+j-1} P_n B' P_n (H_{1,n} - z)^{-j-1}\]

\[= -2 \sum_{j=1}^{m} (H_{2,n} - z)^{-m+j-1}(H_0 - z)^{m-j+1} \times P_n (H_0 - z)^{-m+j-1} B'(H_0 - z)^{-j} P_n \times (H_0 - z)^j(H_{1,n} - z)^{-j}.\]

Referring to Proposition 4.8 we have that \((H_{2,n} - z)^{-m} - (H_{1,n} - z)^{-m} \in L_1(L^2(\mathbb{R}; \mathcal{H}))\).

(ii). Using decompositions (5.1) and (5.3) we see that it is sufficient to prove the convergence of each term separately.

By (5.2), the operator \((H_0 - z)^{-m+j-1} B'(H_0 - z)^{-j} \in L_1(L^2(\mathbb{R}; \mathcal{H}))\) for all \(j = 1, \ldots, m\), and therefore, by Lemma 2.9 we have that

\[P_n (H_0 - z)^{-m+j-1} B'(H_0 - z)^{-j} P_n \xrightarrow{\|\cdot\|_1} (H_0 - z)^{-m+j-1} B'(H_0 - z)^{-j}.\]

In addition, by Proposition 4.10 we have

\[(H_{2,n} - z)^{-m+j-1}(H_0 - z)^{m-j+1} \rightarrow (H_2 - z)^{-m+j-1}(H_0 - z)^{m-j+1}\]

and

\[(H_0 - z)^j(H_{1,n} - z)^{-j} \rightarrow (H_0 - z)^j(H_1 - z)^{-j}, \quad j = 1, \ldots, m,\]

in the strong operator topology. Thus, another appeal to Lemma 2.10 completes the proof. \(\square\)

In conclusion of the present section, we discuss some details of our main assumption, Hypothesis 5.1 for the special path \(\{B(t)\}_{t \in \mathbb{R}}\) defined as follows. Suppose that a positive function \(\theta\) on \(\mathbb{R}\) satisfies

\[\theta \in C_0^\infty(\mathbb{R}), \quad \theta' \in L_1(\mathbb{R}),\]

\[\lim_{t \to -\infty} \theta(t) = 0, \quad \lim_{t \to +\infty} \theta(t) = 1.\]

and assume that \(B_+\) is a \(p\)-relative perturbation of \(A_-\). Introduce then the family \(\{B(t)\}_{t \in \mathbb{R}}\) given by

\[B(t) = \theta(t) B_+.\]

Since \(\theta' \in L_1(\mathbb{R})\) and \(B'(t)(A_- + i)^{-p-1} = \theta'(t) B_+(A_- + i)^{-p-1}\), it follows that the assumptions (ii) and (iii) of Hypothesis 3.1 are satisfied. Furthermore, an argument similar to the proof of [CGK16, Proposition 2.2] guarantees that

\[B'(H_0 - z)^{-m-1} \in L_1(L^2(\mathbb{R}; \mathcal{H}))\]

that is, assumption (iv) of Hypothesis 5.1 is satisfied.
Thus, for the special type of family \( \{ B(t) \}_{t \in \mathbb{R}} = \{ \theta(t) B_+ \}_{t \in \mathbb{R}} \) assumptions (ii), (iii) and (iv) of Hypothesis 5.1 are automatically guaranteed by the assumption (5.4) on \( \theta \) and the fact that \( B_+ \) is a \( p \)-relative trace class perturbation of \( A_- \).

Next, we discuss Hypothesis 5.1 (v). By definition of \( \delta_{H_0} \) (see (4.7)) to check Hypothesis 5.1 (v) we have to consider repeated commutators with \( (1 + H_0)^{1/2} \). However, in general, it is hard to work with these commutators. Therefore, we use below a different type of commutator argument, in which the commutators are more manageable.

We now follow a method introduced in [CGRS14, Section 1.3] using the operator \( \delta \).

**Lemma 5.3.** If \( T \in \bigcap_{j=1}^{2k} \text{dom}(L_{H_0}^j) \) for some \( k \in \mathbb{N} \), then \( T \in \bigcap_{j=1}^{k} \text{dom}(\delta_{H_0}) \).

Next, we want to reduce the commutators with \( H_0 \) to commutators with \( A_-^2 \).

To this end, for a self-adjoint operator \( A \) on \( \mathcal{H} \) we introduce the operator

\[
L_{A^2}^k(T) = (1 + A^2)^{−k/2}[A^2, T]^{(k)}
\]

with domain

\[
\text{dom}(L_{A^2}^k) = \{ T \in \mathcal{B}(\mathcal{H}) : T \text{ dom}(A^j) \subset \text{ dom}(A^j), j = 1, \ldots, k \}
\]

and the operator \( (1 + A^2)^{−k/2}[A^2, T]^{(k)} \) defined on \( \text{ dom}(A^{2k}) \) extends to a bounded operator on \( \mathcal{H} \).

**Proposition 5.4.** Let \( \{ B(t) \}_{t \in \mathbb{R}} \) be as in (5.5) with \( \theta \) satisfying (5.4). If \( B_+ \in \bigcap_{j=1}^{k} \text{ dom}(L_{A_+^2}^j) \), for some \( k \in \mathbb{N} \), then \( B, B' \in \bigcap_{j=1}^{k} \text{ dom}(L_{H_0}^j) \).

**Proof.** We prove the assertion for \( B \) only, as the assertion for \( B' \) can be proved similarly.

Firstly, identifying the Hilbert spaces \( L^2(\mathbb{R}; \mathcal{H}) \) and \( L^2(\mathbb{R}) \otimes H \), we have

\[
H_0 = \frac{d^2}{dt^2} + A_+^2 = \frac{d^2}{dt^2} \otimes 1 + 1 \otimes A_+^2.
\]

Therefore, since \( \theta \in C^\infty_0(\mathbb{R}) \) and \( B_+ \text{ dom}(A_+^j) \subset \text{ dom}(A_+^j), j = 1, \ldots, 2k \), it follows that the operator \( B = M_0 \otimes B_+ \) leaves \( \text{ dom}(H_0^j), j = 1, \ldots, k \), invariant.

Furthermore, on \( \text{ dom}(H_0) \) we have

\[
[H_0, B] = \frac{d^2}{dt^2} \otimes 1, M_0 \otimes B_+ + [1 \otimes A_+^2, M_0 \otimes B_+]
\]

\[
= \frac{d^2}{dt^2}, M_0 \otimes B_+ + M_0 \otimes [A_+^2, \otimes B_+].
\]
Hence, on $\text{dom}(H_0^k)$ we have

$$[H_0, M_0 \otimes B_+]^{(k)} = \sum_{l=0}^{k} \frac{d^2}{dt^2} M_0^{(l)} \otimes [A^2_+, B_+]^{(k-l)}.$$ 

By Lemma 11 it follows that the operator

$$C := \left(1 - \frac{d^2}{dt^2}\right)^{-\frac{3}{2}} \left(1 + A^2_+\right)^{\frac{k-1}{2}} (1 + H_0)^{-k/2}$$

is bounded for any $l = 0, \ldots, k$.

Hence, on $\text{dom}(H_0^k)$ we have

$$L_{H_0}^k(B) = (1 + H_0)^{-k/2} [H_0, M_0 \otimes B_+]^{(k)}$$

$$= (1 + H_0)^{-k/2} \sum_{l=0}^{k} \frac{d^2}{dt^2} M_0^{(l)} \otimes [A^2_+, B_+]^{(k-l)}$$

$$= \sum_{l=0}^{k} C \cdot \left(1 - \frac{d^2}{dt^2}\right)^{-\frac{3}{2}} \frac{d^2}{dt^2} M_0^{(l)} \otimes (1 + A^2_+)^{-\frac{k-l}{2}} [A^2_+, B_+]^{(k-l)}.$$ 

It follows from inclusion (10.3) below (for $n = 1$) that $(1 - \frac{d^2}{dt^2})^{-\frac{3}{2}} \frac{d^2}{dt^2} M_0^{(l)}$ extends to a bounded operator on $L^2(\mathbb{R})$ for any $l = 0, \ldots, k$. By assumption the operator $(1 + A^2_+)^{-k-1/2}[A^2_+, B_+]^{(k-l)}$ extends to a bounded operator on $\mathcal{H}$. Therefore, $L_{H_0}^k(B)$ also extends to a bounded operator on $L^2(\mathbb{R}; \mathcal{H})$, as required. 

We now formulate the Hypothesis 5.5 for the special case when the family $\{B(t)\}_{t \in \mathbb{R}}$ is given by $\{\theta(t) B_+\}_{t \in \mathbb{R}}$.

**Hypothesis 5.5.**

(i) Assume that $A_-$ is self-adjoint on $\text{dom}(A_-) \subseteq \mathcal{H}$ with $\mathcal{H}$ a complex, separable Hilbert space and let $\theta$ satisfy (5.4).

(ii) Suppose that an operator $B_+$ is a $p$-relative trace-class perturbation of $A_-$ for some $p \in \mathbb{N}$, that is

$$B_+(A_- + i)^{-p-1} \in L_1(\mathcal{H}).$$

(iii) Assume also that $B_+ \in \bigcap_{j=1}^{2p} \text{dom}(L_{A_-}^j)$, where the mapping $L_{A_-}^j$ is defined by (5.6).

For convenience, we state the following

**Proposition 5.6.** For the special case when $\{B(t)\}_{t \in \mathbb{R}} = \{\theta(t) B_+\}_{t \in \mathbb{R}}$, Hypothesis 5.5 guarantees that Hypothesis 5.1 is satisfied.

6. THE PRINCIPAL TRACE FORMULA

In this section we prove the fundamental result of the present paper, the principal trace formula (1.2), which states that

$$\text{tr} \left( e^{-tH_2} - e^{-tH_1} \right) = -\left(\frac{1}{\pi}\right)^{1/2} \int_0^1 \text{tr} \left( e^{-tA^2_+ (A_+ - A_-)} \right) ds, \quad t > 0,$$

where $A_+ = A_+ + s(A_+ - A_-), s \in [0,1]$ is the straight line path joining $A_-$ and $A_+$ (see Theorem 6.3). As mentioned in the introduction, the principal trace formula allows us to establish further results for the Witten index (see Section 7 below) and for spectral flow (see Section 8). In fact the results of Sections 7 and 8 are (almost immediate) corollaries of the principal trace formula.
The reader may be puzzled by the occurrence of the straight line path in this principal trace formula (in both versions) when we started with a more general path joining $A_{\pm}$. This puzzle will be resolved in Section 8 when we will establish that the right-hand side of the principal trace formula is independent of the path chosen to join $A_{\pm}$, subject of course to some simple constraints.

Our approach to the proof of the principal trace formula relies on an approximation approach in which we use results already known for the path \( \{A_n(t)\}_{t \in \mathbb{R}} \) of reduced operators

\[
A_n(t) = A_- + P_n B(t) P_n,
\]

where, as before, \( P_n = \chi_{[-n,n]}(A_-) \). We first recall a result from [CGP+17]. The notation \( \text{erf} \) stands for the error function

\[
(6.2) \quad \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2} \, dy, \quad x \in \mathbb{R}.
\]

**Proposition 6.1.** [CGP+17, Example B.6 (ii) and Theorem B.5] For the path \( \{A_n(t)\}_{t \in \mathbb{R}} \) of reduced operators we have that

\[
e^{-tH_{2,n}} - e^{-tH_{1,n}} \in L^1(L^2(\mathbb{R}; \mathcal{H})), \quad \text{erf}(t^{1/2}A_{+,n}) - \text{erf}(t^{1/2}A_-) \in L_1(\mathcal{H})
\]

and the equation

\[
(6.3) \quad \text{tr} \left( e^{-tH_{2,n}} - e^{-tH_{1,n}} \right) = -\frac{1}{2} \text{tr} \left( \text{erf}(t^{1/2}A_{+,n}) - \text{erf}(t^{1/2}A_-) \right),
\]

holds.

**Remark 6.2.** We note that under the assumption of Hypothesis 5.1 one cannot pass to the limit as \( n \to \infty \) in (6.4), in general. Indeed, consider the case, when the operator \( A_- \) is the two-dimensional Dirac operator (see Section 10) and the perturbed operator \( A_+ \) is given by

\[
A_+ = A_- + 1 \otimes M_f, \quad f \in S(\mathbb{R}).
\]

The family \( \{\theta(t) \otimes M_f\}_{t \in \mathbb{R}} \), with \( \theta \) given by (5.4), satisfies Hypothesis 5.1 (see Section 10). However, by [LSVZ17, Theorem 1.2 (i)] we have that the operator

\[
\text{erf}(t^{1/2}A_+) - \text{erf}(t^{1/2}A_-)
\]

is not a trace-class operator.

To overcome the obstacle mentioned in the above remark we firstly use the (noncommutative) Fundamental Theorem of Calculus obtained in Proposition 2.2 applied to the right-hand side of (6.3) and only after that pass to the limit as \( n \to \infty \). Firstly, we rewrite the principal trace formula obtained in Proposition 6.1 for the reduced operators.

**Lemma 6.3.** For the path \( \{A_n(t)\}_{t \in \mathbb{R}} \) of reduced operators we have

\[
(6.4) \quad \text{tr} \left( e^{-tH_{2,n}} - e^{-tH_{1,n}} \right) = -\left( \frac{t}{\pi} \right)^{1/2} \int_0^1 \text{tr} \left( e^{-tA_{s,n}^2}(A_{+,n} - A_-) \right) ds,
\]

where \( A_{s,n} = A_- + s P_n B_+ P_n, \quad s \in [0,1] \).

**Proof.** By Proposition 6.1 we have

\[
\text{tr} \left( e^{-tH_{2,n}} - e^{-tH_{1,n}} \right) = -\frac{1}{2} \text{tr} \left( \text{erf}(t^{1/2}A_{+,n}) - \text{erf}(t^{1/2}A_-) \right).
\]
Thus, (6.6) and (6.7) imply that the assumption of this proposition since $f$ is a Schwartz function.) we obtain that

$$
\frac{1}{2} \text{tr} \left( \text{erf}(t^{1/2}A_{+}) - \text{erf}(t^{1/2}A_{-}) \right) = \left( \frac{t}{\pi} \right)^{1/2} \int_{0}^{1} \text{tr} \left( e^{-tA_{+}^{2}}(A_{+} - A_{-}) \right) ds.
$$

Hence,

$$
\text{tr} \left( e^{-tH_{2,n}} - e^{-tH_{1,n}} \right) = \left( \frac{t}{\pi} \right)^{1/2} \int_{0}^{1} \text{tr} \left( e^{-tA_{+}^{2}}(A_{+} - A_{-}) \right) ds,
$$
as required.

We now ready to prove the principal trace formula in its heat kernel version, which is the main result of this section.

**Theorem 6.4** (The principal trace formula). Assume Hypothesis 5.1. Let $A_{+} = A_{\pm} + s(A_{+} - A_{\pm})$, $s \in [0,1]$, be the straight line path joining $A_{\pm}$ and $A_{+}$. Then for all $t > 0$, we have

$$
\text{tr} \left( e^{-tH_{2}} - e^{-tH_{1}} \right) = \left( \frac{t}{\pi} \right)^{1/2} \int_{0}^{1} \text{tr} \left( e^{-tA_{+}^{2}}(A_{+} - A_{-}) \right) ds.
$$

**Proof.** By Lemma 6.3 we have

$$
\text{tr} \left( e^{-tH_{2,n}} - e^{-tH_{1,n}} \right) = \left( \frac{t}{\pi} \right)^{1/2} \int_{0}^{1} \text{tr} \left( e^{-tA_{+}^{2}}(A_{+} - A_{-}) \right) ds.
$$

We now pass to the limit as $n \to \infty$.

For the left hand side of (6.6), we firstly note that Theorem 6.2 guarantees that the assumptions of Theorem 2.4 are satisfied with $A_{n} = H_{2,n}$, $A = H_{2}$, $B_{n} = H_{1,n}$, $B = H_{1}$. Hence, since the function $f(\lambda) = e^{-t\lambda_{+}^{2}}$, $t > 0$, is a Schwartz function, it follows from Theorem 2.4 that

$$
\lim_{n \to \infty} \text{tr} \left( e^{-tH_{2,n}} - e^{-tH_{1,n}} \right) = \text{tr} \left( e^{-tH_{2}} - e^{-tH_{1}} \right).
$$

For the right hand side of (6.6) by Proposition 2.17 we have

$$
\lim_{n \to \infty} \int_{0}^{1} \text{tr} \left( e^{-tA_{+}^{2}}(A_{+} - A_{-}) \right) ds = \int_{0}^{1} \text{tr} \left( e^{-tA_{+}^{2}}(A_{+} - A_{-}) \right) ds.
$$

Thus, (6.6) and (6.7) imply that

$$
\text{tr} \left( e^{-tH_{2}} - e^{-tH_{1}} \right) = \left( \frac{t}{\pi} \right)^{1/2} \int_{0}^{1} \text{tr} \left( e^{-tA_{+}^{2}}(A_{+} - A_{-}) \right) ds,
$$

which concludes the proof.

**Remark 6.5.** Using a similar argument one can prove the following

$$
\text{tr} \left( (H_{2} - z)^{-k} - (H_{1} - z)^{-k} \right) = -\frac{(2k - 1)!!}{2k(k - 1)!!} \int_{0}^{1} \text{tr} \left( (A_{+}^{2} - z)^{-k/2} (A_{+} - A_{-}) \right) ds,
$$

which gives an alternative proof of the resolvent version of the principal trace formula proved in [CGK16]. The resolvent version of the formula is known to be connected to cyclic homology (see references in [CGK16]).

Our technique may be used to prove trace formulas for a wide class of functions thus going beyond resolvents and heat kernels. However, at this point it is not clear...
that there is a use for formulas for a general class of functions, and so we omit this refinement. ♦

7. The Witten index and the spectral shift function

In this section we move on to the implications for spectral shift functions of the principal trace formula, Theorem 1.14 which provides a relation between the Witten index of the operator $D_A$ and the spectral shift function $\xi(\cdot; A_+, A_-)$. We follow the detailed treatment in [CGL+17]. What is new here compared with earlier work is that the results established in this paper enable us to remove the ‘relatively trace class perturbation assumption’ in [CGLS16a] as well as the ‘relatively Hilbert-Schmidt class perturbation assumption’ in [CGPS19a]. This extension means that the old difficulty, that the only examples for which the Witten index was defined were low dimensional, is removed. In Section 10 we show that our Hypothesis 3.1 permits consideration of differential operators (in particular, Dirac operators) in any dimension uniformly.

We refer the reader to [Ya92] Chapter 8 for the necessary background on spectral shift function and its properties. We start with introduction of the spectral shift functions $\xi(\cdot; A_+, A_-)$ and $\xi(\cdot; H_2, H_1)$.

By Theorem 5.2 we have $(H_2 - z)^{-m} - (H_1 - z)^{-m} \in L^1(L^2(\mathbb{R}; H))$, for all $z \in \mathbb{C}\setminus\mathbb{R}$. Since the operators $H_2, H_1$ are non-negative, the function $\lambda \mapsto (\lambda - z)^{-m}$ is monotone on the spectra of $H_j$, $j = 1, 2$, for any $z < 0$. Hence, it follows from [Ya92] Section 8.9 that there is a spectral shift function $\xi(\cdot; H_2, H_1)$ for the pair $(H_2, H_1)$ that satisfies

$$\xi(\cdot; H_2, H_1) \in L^1(\mathbb{R}; (|\lambda|^{m+1} + 1)^{-1} d\lambda).$$

Since $H_j \geq 0$, $j = 1, 2$, $\xi(\cdot; H_2, H_1)$ may be specified uniquely by requiring that

$$\xi(\lambda; H_2, H_1) = 0, \quad \lambda < 0.$$  

In addition, the trace formula

$$\text{tr} \left( f(H_2) - f(H_1) \right) = \int_{[0, \infty)} f'(\lambda) \xi(\lambda; H_2, H_1) \, d\lambda, \quad f \in S(\mathbb{R})$$

holds.

We introduce now the spectral shift function for the pair $(A_+, A_-)$ using [Ya05]. As the assumption in [Ya05] is that the operators $(A_+ - z)^{-k} - (A_- - z)^{-k}$, $z \in \mathbb{C}\setminus\mathbb{R}$, are trace-class for some odd $k \in \mathbb{N}$ we introduce the notation

$$p_0 = 2\left\lfloor \frac{k}{2} \right\rfloor + 1,$$

so that $p_0$ is always odd and $p_0 = p$ if $p$ is odd itself and $p_0 = p + 1$ otherwise.

By Theorem 2.13 we have that $(A_+ - z)^{-p_0} - (A_- - z)^{-p_0} \in L^1(\mathcal{H})$, and therefore, by [Ya05] Theorem 2.2 there exists a function

$$\xi(\lambda; A_+, A_-) \in L^1(\mathbb{R}; (1 + |\lambda|)^{-p_0-1} d\lambda)$$

such that

$$\text{tr} \left( f(A_+) - f(A_-) \right) = \int_{\mathbb{R}} f'(\lambda) \cdot \xi(\lambda; A_+, A_-) \, d\lambda, \quad f \in S(\mathbb{R}).$$

However the spectral shift function $\xi(\cdot; A_+, A_-)$ introduced above is not unique, in general, and therefore we have to fix one particular spectral shift function, which satisfies (7.4) and (7.5). We do this using [CGL+16a].
Firstly recall that since $B_+$ is a $p$-relative trace-class perturbation, it follows that for any $n \in \mathbb{N}$ we have that $A_{+,n} - A_- = B_{+,n} \in \mathcal{L}_1(\mathcal{H})$ (see (2.13)). Therefore, by [Yaf92, Theorem 8.2.1] there exists a unique spectral shift function
\begin{equation}
\xi(\cdot; A_{+,n}, A_-) \in L^1(\mathbb{R}), \quad n \in \mathbb{N}.
\end{equation}

**Theorem 7.1.** Assume Hypothesis[5.1] There exists a unique spectral shift function $\xi(\cdot; A_+, A_-)$ such that
\begin{equation}
\xi(\cdot; A_+, A_-) = \lim_{n \to \infty} \xi(\cdot; A_{+,n}, A_-)
\end{equation}
in $L^1(\mathbb{R}; (|\nu|^{p_0+1} + 1)^{-1}d\nu)$.

**Proof.** Introduce the path $\{A_+(s)\}_{s \in [0,1]}$ by setting
\begin{align}
A_+(s) &= A_- + \hat{P}_s B_+ \hat{P}_s, \quad \text{dom}(A_+(s)) = \text{dom}(A_-), \quad s \in [0,1], \\
\hat{P}_s &= \chi_{[\frac{1}{s}, \frac{1}{s+1}]}(A_-), s \in [0,1], \quad \hat{P}_1 = I,
\end{align}
in particular,
\begin{align}
A_+(0) &= A_{+,1} (\text{see (3.10)}), \quad A_+(1) = A_+.
\end{align}

Since $B_+ = A_+ - A_-$ is a $p$-relative trace-class perturbation of $A_-$ (see [5.8]), inclusion (2.13) implies that $P_n B_+ P_n \in \mathcal{L}_1(\mathcal{H})$, and therefore $A_+(s) - A_- = \hat{P}_s B_+ \hat{P}_s \in \mathcal{L}_1(\mathcal{H})$ for any $s < 1$. Hence there exists a unique spectral shift function $\xi(\cdot; A_+(s), A_-)$ for the pair $(A_+(s), A_-)$, $s < 1$, satisfying, in particular,
\begin{align}
\xi(\cdot; A_+(s), A_-) \in L^1(\mathbb{R}).
\end{align}

Moreover, in complete analogy to Theorem 2.14 the family $A_+(s)$ depends continuously on $s \in [0,1]$ with respect to the family of pseudometrics $d_{p_0,z}(\cdot, \cdot)$
\begin{equation}
d_{p_0,z}(A, A') = \|(A - iI)^{-p_0} - (A' - iI)^{-p_0}\|_{\mathcal{L}_1(\mathcal{H})}
\end{equation}
for $A, A'$ in the set of self-adjoint operators which are $p_0$-resolvent comparable with respect to $A_-$. (equivalently, $A_+$), that is, $A, A'$ satisfy for all $\zeta \in i\mathbb{R} \setminus \{0\}$,
\begin{align}
[(A - \zeta I)^{-p_0} - (A_- - \zeta I)^{-p_0}] - [(A' - \zeta I)^{-p_0} - (A_- - \zeta I)^{-p_0}] \in \mathcal{L}_1(\mathcal{H}).
\end{align}

Thus, the hypotheses of [CGL+16a, Theorem 4.7] are satisfied and hence we conclude that there exists a unique spectral shift function $\xi(\cdot; A_+(s), A_-)$ for the pair $(A_+(s), A_-)$ depending continuously on $s \in [0,1]$ in the space $L^1(\mathbb{R}; (|\nu|^{p_0+1} + 1)^{-1}d\nu)$, satisfying $\xi(\cdot; A_+(0), A_-) = \xi(\cdot; A_{+,1}, A_-)$.

Taking $s = \frac{n-1}{n}$ we obtain
\begin{align}
\xi(\cdot; A_+, A_-) & \xrightarrow[n \to \infty]{\text{Le}} \xi(\cdot; A_+(1), A_-) = \lim_{s \uparrow 1} \xi(\cdot; A_+(s), A_-) \\
&= \lim_{n \to \infty} \xi(\cdot; A_{+,n}, A_-).
\end{align}

Therefore, $\{\xi(\cdot; A_{+,n}, A_-)\}_{n \in \mathbb{N}}$ converges pointwise a.e. to $\xi(\cdot; A_+, A_-)$ as $n \to \infty$. Since every $\xi(\cdot; A_{+,n}, A_-), \ n \in \mathbb{N}$, is uniquely defined, we can fix uniquely the spectral shift function $\xi(\cdot; A_+, A_-)$ satisfying conditions (7.1).

**Remark 7.2.** Since every $\xi(\cdot; A_{+,n}, A_-), n \in \mathbb{N}$, is uniquely defined, Theorem 7.1 implies that we can fix uniquely the spectral shift function $\xi(\cdot; A_+, A_-)$ satisfying equation (7.1). We adopt this method of fixing the spectral shift function for the remainder of this paper.
Now we move on to the proof of Pushnitski’s formula, which establishes a relation between the spectral shift functions \((A_+, A_-)\) and \((H_2, H_1)\).

**Theorem 7.3.** Assume Hypothesis \([5,4]\). Let \(\xi(\cdot; A_+, A_-)\) be the spectral shift function for the pair \((A_+, A_-)\) fixed in \((7.7)\) and let \(\xi(\cdot; H_2, H_1)\) be the spectral shift function for the pair \((H_2, H_1)\) fixed by equality \((7.2)\). Then for a.e. \(\lambda > 0\) we have

\[
(7.14) \quad \xi(\lambda; H_2, H_1) = \frac{1}{\pi} \int_{-\lambda^{1/2}}^{\lambda^{1/2}} \frac{\xi(t; A_+, A_-) \, dt}{(\lambda - t^2)^{1/2}}
\]

with a convergent Lebesgue integral on the right-hand side of \((7.14)\).

**Proof.** By the principle trace formula for the semigroup difference (see Theorem \([6,4]\)) we have that

\[
\text{tr}(e^{-tH_2} - e^{-tH_1}) = -\left(\frac{t}{\pi}\right)^{1/2} \int_0^1 \text{tr}(e^{-tA_+^2}(A_+ - A_-)) \, ds
\]

for all \(t > 0\). On the right hand side of this formula using \((2.22)\) and \((6.5)\) we have that

\[
\left(\frac{t}{\pi}\right)^{1/2} \int_0^1 \text{tr}(e^{-tA_+^2}(A_+ - A_-)) \, ds
\]

\[
(7.15) \quad \lim_{n \to \infty} \left(\frac{t}{\pi}\right)^{1/2} \int_0^1 \text{tr}(e^{-tA_+^2}(A_+ - A_-)) \, ds
\]

\[
= \lim_{n \to \infty} \frac{1}{2} \text{tr}(\text{erf}(t^{1/2}A_+) - \text{erf}(t^{1/2}A_-))
\]

By Krein’s trace formula \([Yaf92, Theorem 8.3.3]\) and the definition of the error function \([5,2]\) it follows that

\[
(7.16) \quad \frac{1}{2} \text{tr} \left( \text{erf}(t^{1/2}A_+) - \text{erf}(t^{1/2}A_-) \right) = \left(\frac{t}{\pi}\right)^{1/2} \int_{\mathbb{R}} e^{-t s^2} \xi(s; A_+, A_-) \, ds.
\]

Furthermore, referring to Theorem \([1,1]\) we obtain

\[
(7.17) \quad \lim_{n \to \infty} \left(\frac{t}{\pi}\right)^{1/2} \int_{\mathbb{R}} e^{-t s^2} \xi(s; A_+, A_-) \, ds = \left(\frac{t}{\pi}\right)^{1/2} \int_{\mathbb{R}} e^{-t s^2} \xi(s; A_+, A_-) \, ds.
\]

Thus, combining \((7.15)\), \((7.16)\) and \((7.17)\) we conclude that the right-hand side of the principal trace formula can be written as

\[
\left(\frac{t}{\pi}\right)^{1/2} \int_0^1 \text{tr}(e^{-tA_+^2}(A_+ - A_-)) \, ds = \left(\frac{t}{\pi}\right)^{1/2} \int_{\mathbb{R}} e^{-t s^2} \xi(s; A_+, A_-) \, ds.
\]

Since the functions \(s \mapsto e^{-t s}, s \in \mathbb{R}, t > 0\), is a Schwartz function, it follows from Krein’s trace formula \((7.3)\) that

\[
\text{tr}(e^{-tH_2} - e^{-tH_1}) = -t \int_0^\infty \xi(\lambda; H_2, H_1) e^{-t \lambda} \, d\lambda.
\]

Thus,

\[
\int_0^\infty \xi(\lambda; H_2, H_1) e^{-t \lambda} \, d\lambda = \left(\frac{1}{\pi \cdot t}\right)^{1/2} \int_{\mathbb{R}} \xi(s; A_+, A_-) e^{-t s^2} \, ds
\]

\[
(7.18) \quad = \left(\frac{1}{\pi \cdot t}\right)^{1/2} \int_0^\infty \frac{\xi(\sqrt{s}; A_+, A_-) + \xi(-\sqrt{s}; A_+, A_-)}{\sqrt{s}} e^{-t s} \, ds,
\]
where for the last integral we used the substitutions $s \mapsto \sqrt{s}$ and $s \mapsto -\sqrt{s}$ for the integrals on $(0, \infty)$ and on $(-\infty, 0)$, respectively.

Let us denote by $L$ the Laplace transform on $L^1_{loc}(\mathbb{R})$. It is well-known that $L\left(\frac{1}{\sqrt{s}}\right)(t) = \frac{1}{\sqrt{\pi} t}$ (see e.g. [AS64, 29.3.4]). Therefore, introducing

$$
\xi_0(s) := \frac{\xi(\sqrt{s}; A_+, A_-) + \xi(-\sqrt{s}; A_+, A_-)}{\sqrt{s}}, \quad s \in [0, \infty),
$$
equality (7.18) can be rewritten as

$$
L(\xi(\lambda; H_2, H_1))(t) = L\left(\frac{1}{\pi \sqrt{s}}\right)(t) \cdot L(\xi_0(s))(t).
$$

By [ABHN01, Proposition 1.6.4] the right-hand side of the above equality is equal to $L\left(\frac{1}{\pi \sqrt{s}} \ast \xi_0(s)\right)(t)$. Therefore, by the uniqueness theorem for the Laplace transform (see e.g. [ABHN01, Theorem 1.7.3]) we have $\xi(\lambda; H_2, H_1) = \left(\frac{1}{\pi \sqrt{s}} \ast \xi_0(s)\right)(\lambda)$ for a.e. $\lambda \in [0, \infty)$. Thus, for a.e. $\lambda \in [0, \infty)$ we have

$$
\xi(\lambda; H_2, H_1) = \frac{1}{\pi} \int_0^\lambda \frac{1}{\sqrt{\lambda - s}} \xi_0(s) ds
$$

\begin{align*}
&= \frac{1}{\pi} \int_0^\lambda \frac{1}{\sqrt{\lambda - s}} \xi(\sqrt{s}; A_+, A_-) + \xi(-\sqrt{s}; A_+, A_-) ds \\
&= \frac{1}{\pi} \int_0^\lambda \xi(\sqrt{s}; A_+, A_-) ds + \frac{1}{\pi} \int_0^\lambda \xi(-\sqrt{s}; A_+, A_-) ds \\
&= \frac{1}{\pi} \int_{-\sqrt{\lambda}}^{\sqrt{\lambda}} \xi(s; A_+, A_-) ds
\end{align*}

as required. \hfill \square

Having established Pushnitski’s formula, we can now prove Theorem [1.1] which provides a relation between the Witten index of the operator $D_A$ and the spectral shift function $\xi(\cdot; A_+, A_-)$. We start with definition of the Witten index.

**Definition 7.4.** Let $T$ be a closed, linear, densely defined operator acting in $\mathcal{H}$ and suppose that for some $t_0 > 0$

$$
e^{-t_0 T^* T} - e^{-t_0 T T^*} \in \mathcal{L}_1(\mathcal{H}).
$$

Then $\left(e^{-t T^* T} - e^{-t T T^*}\right) \in \mathcal{L}_1(\mathcal{H})$ for all $t > t_0$, and one introduces the (semigroup) regularized Witten index $W_s(T)$ of $T$

$$
W_s(T) = \lim_{t \uparrow \infty} \text{tr}_\mathcal{H} \left(e^{-t T^* T} - e^{-t T T^*}\right),
$$

whenever the limit exists.

Recall that for a closed densely defined operator the Witten index has also a different regularisation by resolvent differences (see [BGG+17, CGP+17]). Namely, suppose that for some (and hence for all) $z \in \mathbb{C}\setminus[0, \infty)$, we have that

$$
[(T^* T - z)^{-1} - (T T^* - z)^{-1}] \in \mathcal{L}_1(\mathcal{H}).
$$

Then the resolvent regularized Witten index $W_r(T)$ of $T$ is defined by

$$
W_r(T) = \lim_{\lambda \uparrow 0} (-\lambda) \text{tr} \left( (T^* T - \lambda)^{-1} - (T T^* - \lambda)^{-1} \right)
$$

(7.21)
whenever this limit exists.

However, in our setting we aim to consider the case when $T$ is a differential type operator. In this case, it is typical that the difference of resolvents $(T^* T - z)^{-1} - (TT^* - z)^{-1}$ belongs to a higher Schatten class as would be expected for the study of differential operators in higher dimensions. Therefore, we need to modify the definition of resolvent regularisation of the Witten index.

**Definition 7.5.** Let $T$ be a closed, linear, densely defined operator acting in $\mathcal{H}$ and let $k \in \mathbb{N}$. Suppose that for all $\lambda < 0$ we have that
\[
[(T^* T - \lambda)^{-k} - (TT^* - \lambda)^{-k}] \in \mathcal{L}_1(\mathcal{H}).
\]
Then the $k$-th resolvent regularized Witten index $W_{k,r}(T)$ of $T$ is defined by
\[
W_{k,r}(T) = \lim_{\lambda \uparrow 0} (\lambda)^k \tr ((T^* T - \lambda)^{-k} - (TT^* - \lambda)^{-k})
\]
whenever this limit exists.

**Remark 7.6.** We note that the $k$-th resolvent regularised Witten index is the limit (as $\lambda \uparrow 0$) of the so-called homological index (see [CGK15, CGK16]).

To establish our results for resolvent regularisations of the Witten index we also need the following lemma, which establishes a more general version of Lemma 4.1 (iii). Its proof is a verbatim repetition of the argument of Lemma 4.1 (iii) and is therefore omitted.

**Lemma 7.7.** Let $k \in \mathbb{N}$. Introduce the linear operator
\[
T_k : L^1((0, \infty); (\nu + 1)^{-k-1} \, d\nu) \to L^1_{\text{loc}}((0, \infty); \, d\lambda)
\]
by setting
\[
(T_k f)(\lambda) = -k\lambda^k \int_0^\infty (\nu + \lambda)^{-k-1} f(\nu) \, d\nu, \quad \lambda > 0.
\]
If $0$ is a Lebesgue point for $f \in L^1((0, \infty); (\nu + 1)^{-k-1} \, d\nu)$, then
\[
\lim_{\lambda \downarrow 0} (T_k f)(\lambda) = f_L(0_+).
\]

We are now in a position to state our main result in this present Section. Its proof closely follows the argument used in [CGP+17].

**Theorem 7.8.** Assume Hypothesis [7.7] and assume that $0$ is a right and a left Lebesgue point of $\xi(\cdot; A_+, A_-)$. Then $0$ is a right Lebesgue point of $\xi(\cdot; H_2, H_1)$
\[
\xi_L(0_+; H_2, H_1) = \frac{\xi_L(0_+; A_+, A_-) + \xi_L(0_-; A_+, A_-)}{2}
\]
and the Witten indices $W_s(D_A)$ and $W_{k,r}(D_A)$, $k \geq m$, exist and equal
\[
W_s(D_A) = W_{k,r}(D_A) = \frac{\xi_L(0_+; H_2, H_1)}{2} = \frac{\xi_L(0_+; A_+, A_-) + \xi_L(0_-; A_+, A_-)}{2}
\]

**Proof.** First, one rewrites (7.14) in the form,
\[
\xi(\lambda; H_2, H_1) = \frac{1}{\pi} \int_0^{\lambda/2} \frac{d\nu}{(\lambda - \nu^2)^{1/2}} \left[ \xi(\nu; A_+, A_-) + \xi(-\nu; A_+, A_-) \right], \quad \lambda > 0.
\]
Define the function $f(\nu) = \left[ \xi(\nu; A_+, A_-) + \xi(-\nu; A_+, A_-) \right] / 2$. By assumption, $0$ is a right and a left Lebesgue point of $\xi(\cdot; A_+, A_-)$, and therefore, $0$ is a right Lebesgue
point of $f$. Equality \[7.20\] together with [CGP+17, Lemma 4.1 (i)] implies that $0$ is a right Lebesgue point of $\xi(\cdot; H_2, H_1)$ and

$$
\xi_L(0_+; H_2, H_1) = \frac{1}{2} \ell_L(0_+) = \frac{1}{2} (\xi_L(0_+; A_+, A_-) + \xi_L(0_-; A_+, A_-)).
$$

Next, to prove the equality for the semigroup regularised Witten index $W_s(D_A)$ we introduce the function

$$
\Xi(r; H_2, H_1) = \int_0^r \xi(s; H_2, H_1) \, ds, \quad r > 0.
$$

By Krein’s trace formula (7.3) we have that

$$
\frac{1}{t} \text{tr} (e^{-tH_2} - e^{-tH_1}) = - \int_0^\infty \xi(s; H_2, H_1) e^{-ts} \, ds = - \int_0^\infty e^{-ts} \Xi(s; H_2, H_1).
$$

We have already established, that $0$ is a right Lebesgue point of $\xi(\cdot; H_2, H_1)$. Hence, one obtains that

$$
\lim_{r \downarrow 0^+} \frac{\Xi(r; H_2, H_1)}{r} = \Xi'(0_+; H_2, H_1) = \xi_L(0_+; H_2, H_1)
$$

exists. Then, an Abelian theorem for Laplace transforms [Wid41, Theorem 1, p. 181] (with $\gamma = 1$) implies that

$$
- \lim_{t \to \infty} \text{tr}_H (e^{-tH_2} - e^{-tH_1}) = \lim_{r \downarrow 0^+} \frac{\Xi(r; H_2, H_1)}{r} = \xi_L(0_+; H_2, H_1).
$$

To prove the equality for the $k$-th resolvent regularisation $W_{k,r}(D_A)$ we write

$$
W_{k,r}(D_A) = \lim_{\lambda \downarrow 0^+} (-\lambda)^k \text{tr} \left( (H_2 - \lambda)^{-k} - (H_1 - \lambda)^{-k} \right)
$$

$$
= -k \lim_{\lambda \downarrow 0^+} \int_0^\infty (\nu - \lambda)^{-k-1} \xi(\nu; H_2, H_1) \, d\nu
$$

$$
= \lim_{\lambda \downarrow 0^+} (T_k \xi(\cdot; H_2, H_1))(\nu),
$$

where $T_k$ is the operator introduced in Lemma [43]. Since $0$ is a right Lebesgue point for $\xi(\cdot; H_2, H_1) \in L^1((0, \infty); (\nu + 1)^{-k-1} \, d\nu)$, $k \geq m$, Lemma [7.7] implies that

$$
W_{k,r}(D_A) = \xi_L(0_+; H_2, H_1) = \frac{1}{2} (\xi_L(0_+; A_+, A_-) + \xi_L(0_-; A_+, A_-)),
$$

as required.

\[ \square \]

8. Spectral flow

In this section we establish the connection of the Witten index of the operator $D_A$ to the spectral flow along the path $\{A(t)\}_{t \in \mathbb{R}}$ in the special case when $A_\pm$ are Fredholm operators and so the spectral flow $\text{sf}\{A(t)\}_{t \in \mathbb{R}}$ is well-defined. This provides an extension of the Robbin-Salamon result to the situation where the endpoints of the path are not invertible (see also [CGK16]) so that $D_A$ is not Fredholm.

Throughout this section we assume the following:
Hypothesis 8.1. In addition to Hypothesis 5.1, we assume that the asymptotes \( A_{\pm} \) of the path \( \{A(t)\}_{t \in \mathbb{R}} \) are Fredholm.

We recall the analytical definition of the spectral flow due to J. Phillips [Phi96]. Let \( \chi \) be the characteristic function of the interval \([0, \infty)\) and let \( \{F_t\}_{t \in [0,1]} \) be a norm continuous path of bounded self-adjoint Fredholm operators on \( \mathcal{H} \). Denote by \( \pi \) the projection onto the Calkin algebra \( \mathcal{B}(\mathcal{H})/\mathcal{K}(\mathcal{H}) \). Then one may show that 
\[
\pi(\chi(F_t)) = \pi(\chi(F_0)).
\]
Since the spectra of \( \pi(F_t) \) are bounded away from 0, this latter path is continuous. By compactness we can choose a partition \( 0 = t_0 < t_1 < \cdots < t_k = b \) so that for each \( i = 1, 2, \ldots, k \) we have the inequality
\[
\|\pi(\chi(F_s)) - \pi(\chi(F_t))\| < 1/2 \quad \text{for all } t, s \in [t_{i-1}, t_i].
\]
Letting \( P_i = \chi(F_{t_i}) \) for \( i = 0, 1, \ldots, k \), then by the previous inequality (see [6]) the operator \( P_{i-1}P_i : P_{i} \mathcal{H} \to P_{i-1} \mathcal{H} \) is Fredholm. Then we define the spectral flow along the path \( \{F_t\}_{t \in [0,1]} \) to be the number:
\[
\text{sf}(\{F_t\}_{t \in [0,1]}) = \sum_{i=1}^{k} \text{index}(P_{i-1}F_i).
\]

The main results of [Phi96] show that this analytic notion is well defined being independent of the partition into ‘small’ intervals and that it reproduces the usual topological point of view.

Our definition of a Fredholm operator \( S \) in the unbounded self-adjoint case exploits the Riesz map \( g : S \to S(1 + S^2)^{-1/2} \), so that we say \( S \) is Fredholm if its image under this map is a bounded Fredholm operator. A path of unbounded Fredholm operators \( \{S(t)\}_{t \in [0,1]} \) is continuous if the path of bounded transforms \( \{g(S(t))\}_{t \in [0,1]} \) is continuous. Then the spectral flow along \( \{S(t)\}_{t \in [0,1]} \) is defined via Phillips’ definition to be the spectral flow along the bounded path \( \{g(S(t))\}_{t \in [0,1]} \).

The analytic formulas for spectral flow that we will exploit require us to introduce differentiable paths of unbounded Fredholm operators. In the following definition we use a neutral notation in order that later the definition may be applied in different contexts.

Definition 8.2. (i) A path \( \{D(t)\}_{t \in [0,1]} \) of unbounded self-adjoint operators is called \( \Gamma \)-differentiable at the point \( t = t_0 \) if and only if there is a bounded linear operator \( G \) such that
\[
\lim_{t \to t_0} \frac{D(t) - D(t_0)}{t} (1 + D(t_0)^2)^{-1/2} - G \bigg|_{\mathcal{B}(\mathcal{H})} = 0.
\]
In this case, we set \( \dot{D}(t_0) = G(1 + D(t_0)^2)^{1/2} \). By [CPS09] Lemma 25 the operator \( \dot{D}(t) \) is a symmetric linear operator with the domain \( \text{dom}(\dot{D}(t)) \).
(ii) If the mapping \( t \to \dot{D}(t)(1 + D(t)^2)^{-1/2} \), \( t \in [0,1] \), is defined and continuous with respect to the operator norm, then the path \( \{D(t)\}_{t \in [0,1]} \) is called continuously \( \Gamma \)-differentiable or a \( C^1_{\Gamma} \)-path.

We will mainly focus on spectral flow along a \( C^1_{\Gamma} \)-path \( \{D_t\}_{t \in [0,1]} \) of self-adjoint unbounded Fredholm operators and using [CPS09] Theorem 22 we define this as
\[(8.1) \quad \text{sf}(\{D_t\}_{t \in [0,1]}) := \text{sf}(\{g(D_t)\}_{t \in [0,1]}).
\]
We state now a particularly useful formula from [CPS09] for the spectral flow. This formula will allow us to use again the approximation argument.
Theorem 8.3. [CPS09, Theorem 9] Let \( \{D_t\}_{t \in [0,1]} \) be a \( C^1 \)-path of (unbounded) self-adjoint Fredholm operators joining endpoints \( D_0, D_1 \). Suppose that

(i) \( \int_0^1 \|D_t e^{-\lambda D^2_t}\|_1 dt < \infty, \lambda > 0; \)
(ii) The operator \( \frac{1}{2 \lambda} \text{erf}(\lambda^{1/2} D_1) - \frac{1}{2 \lambda} \text{erf}(\lambda^{1/2} D_0) - [\chi_{[0,\infty)}(D_1) - \chi_{[0,\infty)}(D_0)] \)

is a trace-class operator.

Then

\[
\text{sf}(\{D_t\}_{t \in [0,1]}) = \int_0^1 \text{tr} (D_t e^{-\lambda D^2_t}) dt
+ \text{tr} \left( \frac{1}{2} \text{erf}(\lambda^{1/2} D_1) - \frac{1}{2} \text{erf}(\lambda^{1/2} D_0) - [\chi_{[0,\infty)}(D_1) - \chi_{[0,\infty)}(D_0)] \right).
\]

To prove that the spectral flow \( \text{sf}(\{A(t)\}) \) is well-defined we need to show that the path \( \{A(t)\}_{t \in \mathbb{R}} \) is continuous in an appropriate topology. To do this, we first note that Lemma 2.7 together with the Hölder inequality immediately imply the following

Lemma 8.4. Assume Hypothesis \[3.7\]. We have that

\[
B'(t)(A_- + i)^{-1} \in L_{p+1}(\mathcal{H}), \quad \int_{\mathbb{R}} \|B'(t)(A_- + i)^{-1}\|_{p+1} dt < \infty.
\]

Repeating the proof of [GLM+11, Remark 3.3] we obtain that

\[
(8.2) \quad B(t)(|A_-| + 1)^{-1} = \int_{-\infty}^{t} B'(s)(|A_-| + 1)^{-1} ds \in L_{p+1}(\mathcal{H}), \quad t \in \mathbb{R}
\]

and

\[
(8.3) \quad B'_+(|A_-| + 1)^{-1} = \int_{-\infty}^{\infty} B'(s)(|A_-| + 1)^{-1} ds \in L_{p+1}(\mathcal{H}).
\]

In order to relate the Witten index to spectral flow we will again use our approximation method, that is, as before (see Section \[3\]), we introduce the family

\[
A_n(t) = A_- + P_n B(t) P_n, \quad t \in \mathbb{R}, \quad A_{-n} = A_-, \quad A_{+n} = A_- + P_n B_+ P_n,
\]

where \( P_n = \chi_{[-n,n]}(A_-) \).

The key ingredient of our argument is Theorem \[8.3\] and that result defines the spectral flow for a path \( \{S(t)\}, t \in [0,1] \), in the parametrised norm, to avoid confusion. Let \( r : [0,1] \to \mathbb{R} \) be a continuously differentiable strictly increasing function. Introduce the path \( \{S(t)\}_{t=0}^{1} \) by letting

\[
(8.4) \quad S(0) = A_-, \quad S(t) = A(r(t)), \quad t \in (0,1), \quad S(1) = A_+,
\]

and the corresponding path of ‘cut-off’ operators \( \{S_n(t)\}_{t=0}^{1} \) by

\[
(8.5) \quad S_n(0) = A_-, \quad S_n(t) = A_n(r(t)), \quad t \in (0,1), \quad S_n(1) = A_{+n},
\]

Recall that Theorem \[8.3\] is established for a \( C^1 \)-path of unbounded Fredholm operators (see Definition \[8.2\] for the precise definition of a \( C^1 \)-path). Therefore, we begin by showing that both the paths \( \{A(t)\}_{t=-\infty}^{+\infty}, \{A_n(t)\}_{t=-\infty}^{+\infty} \) (and equivalently, \( \{S(t)\}_{t=0}^{1} \) and \( \{S_n(t)\}_{t=0}^{1} \)) have the necessary regularity.

Lemma 8.5. The paths \( \{S(t)\}_{t \in [0,1]} \) and \( \{S_n(t)\}_{t \in [0,1]} \) are \( C^1 \)-paths of self-adjoint Fredholm operators.
Thus, we only need to show that 3.2 states that $B(t)$, $t \in \mathbb{R}$, is an $A_-$-relatively compact operators. Hence by Proposition 2.8 we have that $A(t) = A_- + B(t), t \in \mathbb{R}$, has the same essential spectra as $A_-$, which by Hypothesis 3.1 implies that $A(t), t \in \mathbb{R}$, are Fredholm operators.

Next, we show that $\{S(t)\}_{t \in [0, 1]}$ is a $C^1_t$-path. By Hypothesis 5.1 we have that $\{S(t)\}_{t \in [0, 1]}$ is $\Gamma$-differentiable at any point and $\dot{S}(t) = A'(r(t)) \cdot r'(t) = B'(r(t)) \cdot r'(t)$. Next for arbitrary $t_1, t_2 \in [0, 1]$ we have

$$
\|\dot{S}(t_1)(1 + S(t_1)^2)^{-1/2} - \dot{S}(t_2)(1 + S(t_2)^2)^{-1/2}\|
\leq \|B'(r(t_1)) - B'(r(t_2))\|\|(1 + S(t_1)^2)^{-1/2} - (1 + S(t_2)^2)^{-1/2}\|
\quad + \|B'(r(t_2))\|\|(1 + S(t_1)^2)^{-1/2} - (1 + S(t_2)^2)^{-1/2}\|.
$$

By the assumption the family $\{B(t)\}_{t \in [0, 1]}$ is continuously differentiable with respect to the uniform norm. Since the function $r$ is continuous, we obtain that $\|B'(r(t_1)) - B'(r(t_2))\| \to 0$ as $t_1 \to t_2$. In addition, we have

$$(1 + S(t_1)^2)^{-1/2} - (1 + S(t_2)^2)^{-1/2}
= \frac{1}{\pi} \int_0^\infty d\lambda \lambda^{-1/2}((1 + \lambda + S(t_1)^2)^{-1} - (1 + \lambda + S(t_2)^2)^{-1}).$$

Using the resolvent identity and continuity of the path $\{B(t)\}_{t \in [0, 1]}$ one can conclude that $\|(1 + S(t_1)^2)^{-1/2} - (1 + S(t_2)^2)^{-1/2}\| \to 0$ as $t_1 - t_2 \to 0$.

Thus, $\|\dot{S}(t_1)(1 + S(t_1)^2)^{-1/2} - \dot{S}(t_2)(1 + S(t_2)^2)^{-1/2}\| \to 0$ as $t_1 - t_2 \to 0$, which proves that the mapping $t \mapsto \dot{S}(t)(1 + S(t)^2)^{-1/2}$ is continuous, and hence, concludes the proof.

Thus, by Lemma 5.1 both $\{A(t)\}_{t \in [0, 1]}$ and $\{A_n(t)\}_{t \in [0, 1]}$ are $C^1_t$-paths of Fredholm operators. Therefore, by 3.1 we can define the spectral flow for both paths $\{A(t)\}_{t \in [0, 1]}$ and $\{A_n(t)\}_{t \in [0, 1]}$ by setting

$$\text{sf}(\{A(t)\}_{t \in [0, 1]}) := \text{sf}(\{S(t)\}_{t = 0}^1) = \text{sf}(\{g(S(t))\}_{t = 0}^1)$$
and

$$\text{sf}(\{A_n(t)\}_{t \in [0, 1]}) := \text{sf}(\{S_n(t)\}_{t = 0}^1) = \text{sf}(\{g(S_n(t))\}_{t = 0}^1).$$

At this point in the argument we want to apply Theorem 8.3. For this result we need to check the hypotheses as follows.

**Lemma 8.6.** The path $\{S_n(t)\}_{t = 0}^1$ satisfies the assumptions of Theorem 8.3.

**Proof.** By Lemma 8.3 the path $\{S_n(t)\}_{t \in [0, 1]}$ is a $C^1 t$-path. Moreover, $\dot{S}_n(t) = P_nB'(r(t))P_n$, which implies that $\dot{S}_n(t)$ is a trace-class operator for any $t \in [0, 1]$ (see 2.13). Hence assumption (i) of Theorem 8.3 is satisfied.

Next, by Proposition 6.1 we have that

$$\frac{1}{2} \text{erf}(t^{1/2}A_{+n}) - \frac{1}{2} \text{erf}(t^{1/2}A_-) \in \mathcal{L}_1(\mathcal{H}).$$

Thus, we only need to show that

$$\chi_{[0, \infty)}(A_{+n}) - \chi_{[0, \infty)}(A_-) \in \mathcal{L}_1(\mathcal{H}).$$
Since 0 is an isolated eigenvalue of \( A_{+,n} \) and \( A_- \), there exists \( \varepsilon > 0 \), such that 
\[
\chi_{(0,\varepsilon)}(A_{+,n}) = \chi_{(0,\varepsilon)}(A_-) = 0 \quad \text{and} \quad \varepsilon \notin \sigma(A_{+,n}), \sigma(A_-).
\]
Therefore,
\[
\begin{align*}
\chi_{[0,\infty)}(A_{+,n}) - \chi_{[0,\infty)}(A_-) & = -[\chi_{(-\infty,0)}(A_{+,n}) - \chi_{(-\infty,0)}(A_-)] \\
& = -[\chi_{(-\infty,-\varepsilon)}(A_{+,n}) - \chi_{(-\infty,-\varepsilon)}(A_-)] \\
& = -[\chi_{(-\infty,0)}(A_{+,n} - \varepsilon) - \chi_{(-\infty,0)}(A_- - \varepsilon)].
\end{align*}
\]  

(8.8)

Introduce a smooth cut-off function \( \varphi \in C^\infty(\mathbb{R}) \) satisfying
\[
\varphi(\nu) = \begin{cases} 
1, & \nu \leq -\nu_0, \\
0, & \nu \geq \nu_0,
\end{cases} \quad \text{and} \quad \int_{-\nu_0}^{\nu_0} \varphi'(\nu) d\nu = -1,
\]
for some \( \nu_0 > 0 \). Since \( (A_{+,n} - \varepsilon) - (A_- - \varepsilon) = A_{+,n} - A_- \in \mathcal{L}_1(\mathcal{H}) \), and \( \phi \in C^\infty(\mathbb{R}) \) with \( \phi' \in L_1(\mathbb{R}) \), it follows that
\[
\phi(A_{+,n} - \varepsilon) - \phi(A_- - \varepsilon) \in \mathcal{L}_1(\mathcal{H}).
\]

(8.10)

Note that \( \varphi \) coincides with the characteristic function of the interval \((-\infty,0)\) on the spectra of \( A_{+,n} - \varepsilon \) and \( A_- - \varepsilon \), and therefore
\[
\chi_{(-\infty,0)}(A_{+,n} - \varepsilon) = \phi(A_{+,n} - \varepsilon), \quad \chi_{(-\infty,0)}(A_- - \varepsilon) = \phi(A_- - \varepsilon).
\]

Hence, combining (8.8) and (8.10), we infer that
\[
\begin{align*}
\chi_{[0,\infty)}(A_{+,n}) - \chi_{[0,\infty)}(A_-) & = [\chi_{(-\infty,0)}(A_{+,n} - \varepsilon) - \chi_{(-\infty,0)}(A_- - \varepsilon)] \\
& = -[\phi(A_{+,n} - \varepsilon) - \phi(A_- - \varepsilon)] \in \mathcal{L}_1(\mathcal{H}),
\end{align*}
\]

which suffices to conclude the proof.

\[\square\]

The next step of our approach is to give a formula, similar to that of [ACS07], relating the spectral flow along the path \( \{A_n(t)\}_{t=\infty}^{\infty} \) and the spectral shift function \( \xi(\cdot; A_{+,n}, A_-) \). To this end, we recall (see (7.11)) that for each \( n \in \mathbb{N} \) there exists a (unique) spectral shift function \( \xi(\cdot; A_{+,n}, A_-) \) for the pair \( (A_{+,n}, A_-) \). By Proposition 8.3, the operators \( A_{+,n} \) and \( A_- \) are Fredholm, and therefore, it follows from the properties of the spectral shift function (see e.g. [Ya92 Proposition 8.2.8]) that, for every \( n \in \mathbb{N} \), the function \( \xi(\cdot; A_{+,n}, A_-) \) is left and right continuous at zero and
\[
(8.11) \quad \xi(0+; A_{+,n}, A_-) - \xi(0-; A_{+,n}, A_-) = \dim \ker(A_-) - \dim \ker(A_{+,n}).
\]

The next proposition is the first step in the proof of our formula for the Witten index in terms of spectral flow. This formula connects the spectral flow \( \text{sf}(\{A_n(t)\}_{t=\infty}^{\infty}) \) to the spectral shift function \( \xi(\cdot; A_{+,n}, A_-) \). The main ingredient of our argument is Theorem 8.3.

**Proposition 8.7.** Let \( A_{+,n}, \{A_n(t)\}_{t=\infty}^{\infty} \) and \( \{S_n(t)\}_{t \in [0,1]} \) be as before. Then for the spectral flow \( \text{sf}(\{A_n(t)\}_{t=\infty}^{\infty}) \), defined by (8.7) we have
\[
\text{sf}(\{A_n(t)\}_{t=\infty}^{\infty}) = \frac{1}{2} [\xi(0+; A_{+,n}, A_-) + \xi(0-; A_{+,n}, A_-)] \\
+ \frac{1}{2} [\dim(\ker(A_{+,n})) - \dim(\ker(A_-))].
\]
Lemma 8.6. By (8.8) we have

\[ \text{(8.12)} \]

Proof. By Lemma 8.6 the path \( \{S_n(t)\}_{t \in [0,1]} \) satisfies the assumption of Theorem 8.3. Hence, by the result of this theorem

\[
\text{sf}((\{A_n(t)\}_{t = -\infty}^\infty) = \text{sf}((\{S_n(t)\}_{t \in [0,1]})
\]

\[ = \int_0^1 \text{tr} ((A_{t,n} - A_-) e^{-\lambda A_t^2(r(t)))} dt + \frac{1}{2} \text{tr}[\text{erf}(\lambda^{1/2}A_{t,n}) - \text{erf}(\lambda^{1/2}A_-)]
\]

\[- \text{tr}[\chi_{[0,\infty)}(A_{t,n}) - \chi_{[0,\infty)}(A_-)].
\]

By Proposition 2.2 we have

\[
\int_0^1 \text{tr} ((A_{t,n} - A_-) e^{-\lambda A_t^2(r(t)))} dt = \frac{1}{2} \text{tr}[\text{erf}(\lambda^{1/2}A_{t,n}) - \text{erf}(\lambda^{1/2}A_-)],
\]

and therefore

\[
\text{sf}((\{A_n(t)\}_{t = -\infty}^\infty) = \text{tr}[\text{erf}(\lambda^{1/2}A_{t,n}) - \text{erf}(\lambda^{1/2}A_-)]
\]

\[- \text{tr}[\chi_{[0,\infty)}(A_{t,n}) - \chi_{[0,\infty)}(A_-)].
\]

We now compute \( \text{tr}[\chi_{[0,\infty)}(A_{t,n}) - \chi_{[0,\infty)}(A_-)] \). Fix \( \varepsilon > 0 \) as in the proof of Lemma 8.6. By (8.3) we have

\[ (8.12) \]

\[
\text{tr} [\chi_{[0,\infty)}(A_{t,n}) - \chi_{[0,\infty)}(A_-)] = - \text{tr} [\chi_{(-\infty,0)}(A_{t,n}) - \chi_{(-\infty,0)}(A_-)].
\]

Introducing the family \( \tilde{B}_n(t) = B_n(t) - \varepsilon \), we have \( \tilde{B}_n(t) = B_n'(t) \) for all \( t \in \mathbb{R} \), and hence the family \( \{\tilde{B}_n(t)\}_{t \in \mathbb{R}} \) satisfies the conditions of [GLM11] relative to \( A_- - \varepsilon \). In addition, for the corresponding asymptotes \( A_{t,n} - \varepsilon, A_- - \varepsilon \), 0 is not in their spectra and \( (A_{t,n} - \varepsilon) - (A_- - \varepsilon) = A_{t,n} - A_- \in \mathcal{L}_1(\mathcal{H}) \). Hence, by [GLM11] Lemma 7.5] we have

\[
\text{tr}[\chi_{(-\infty,0)}(A_{t,n}) - \chi_{(-\infty,0)}(A_-)] = - \xi(0; A_{t,n} - \varepsilon, A_- - \varepsilon),
\]

which implies that

\[ (8.13) \]

\[
\text{tr}[\chi_{[0,\infty)}(A_{t,n}) - \chi_{[0,\infty)}(A_-)] = \xi(0; A_{t,n} - \varepsilon, A_- - \varepsilon) = \xi(\varepsilon; A_{t,n}, A_-).
\]

Thus, combining (8.12) with (8.13) we conclude that

\[
\text{sf}((\{A_n(t)\}_{t = -\infty}^\infty) = \text{tr}[\text{erf}(\lambda^{1/2}A_{t,n}) - \text{erf}(\lambda^{1/2}A_-)] - \xi(\varepsilon; A_{t,n}, A_-).
\]

Next, we take the limit as \( \lambda \to \infty \). Firstly, by Proposition 6.1 we have

\[
\text{sf}((\{A_n(t)\}_{t = -\infty}^\infty) = -2 \lim_{\lambda \to \infty} \text{tr}(e^{-\lambda H_{2,n}} - e^{-\lambda H_{1,n}}) - \xi(\varepsilon; A_{t,n}, A_-).
\]

Using [CGP17] Theorem 4.3 it follows that

\[
-2 \lim_{\lambda \to \infty} \text{tr}(e^{-\lambda H_{2,n}} - e^{-\lambda H_{1,n}}) = 2W_s(D_{A_n})
\]

\[ = [\xi(0_+; A_{t,n}, A_-) + \xi(0_-; A_{t,n}, A_-)].
\]

Therefore, since \( \xi(\varepsilon; A_{t,n}, A_-) = \xi(0_+; A_{t,n}, A_-) \), we have

\[
\text{sf}((\{A_n(t)\}_{t = -\infty}^\infty) = [\xi(0_+; A_{t,n}, A_-) + \xi(0_-; A_{t,n}, A_-)] - \xi(\varepsilon; A_{t,n}, A_-)
\]

\[ = \frac{1}{2} [\xi(0_+; A_{t,n}, A_-) + \xi(0_-; A_{t,n}, A_-)]
\]

\[- \frac{1}{2} [\xi(0_+; A_{t,n}, A_-) - \xi(0_-; A_{t,n}, A_-)].
\]
Referring to (8.11) we now see that
\[
\text{sf}(\{A_n(t)\}_{t=-\infty}^\infty) = \frac{1}{2}[\xi(0_+; A_{+,n}, A_-) + \xi(0_-; A_{+,n}, A_-)]
+ \frac{1}{2}[\dim(\ker(A_{+,n})) - \dim(\ker(A_-))],
\]
which concludes the proof. □

Having established the desired formula for the reduced operators we now want to pass to the limit as \( n \to \infty \). We state some of the necessary approximation results in separate lemmas. The first step is to prove that the kernel of the operator \( A_{+,n} \) has the same dimension as the kernel of \( A_+ \) for sufficiently large \( n \in \mathbb{N} \).

**Lemma 8.8.** For sufficiently large \( n \in \mathbb{N} \) we have that
\[
\dim(\ker(A_{+,n})) = \dim(\ker(A_+)).
\]

**Proof.** By Theorem 2.13 we have
\[
\|(A_{+,n} - i)^{-1} - (A_+ - i)^{-1}\|_\infty \leq \|(A_{+,n} - i)^{-1} - (A_+ - i)^{-1}\|_{p+1}
= \left\| \left( (A_{+,n} - i)^{-1} - (A_- - i)^{-1} \right) \left( (A_+ - i)^{-1} - (A_- - i)^{-1} \right)^\dag \right\|_{p+1} \to 0
\]
as \( n \to \infty \). That is, \( A_{+,n} \to A_+ \) in the norm resolvent sense. Therefore, by [RS80, Theorem VIII.23 (i)] we obtain that 0 is an isolated eigenvalue of \( \sigma(A_{+,n}) \) for sufficiently large \( n \in \mathbb{N} \). In addition, by [RS80, Theorem VIII.23 (ii)] for sufficiently small \( \varepsilon > 0 \) we have that \( \| \chi_{(-\varepsilon,\varepsilon)}(A_{+,n}) - \chi_{(-\varepsilon,\varepsilon)}(A_+) \| \to 0 \). Therefore, for sufficiently large \( n \in \mathbb{N} \), the rank of \( \chi_{(-\varepsilon,\varepsilon)}(A_{+,n}) \) equals the rank of \( \chi_{(-\varepsilon,\varepsilon)}(A_+) \), that is for sufficiently large \( n \in \mathbb{N} \) the multiplicity of 0 for \( A_{+,n} \) is the same as multiplicity for \( A_+ \). □

Next, we handle the approximation of spectral flow.

**Lemma 8.9.** For \( n \) sufficiently large we have
\[
(8.14) \quad \text{sf}(\{A(t)\}_{t=-\infty}^\infty) = \text{sf}(\{A_n(t)\}_{t=-\infty}^\infty).
\]

**Proof.** By (8.10) we have that \( \text{sf}(\{A(t)\}_{t=-\infty}^\infty) = \text{sf}(\{g(S(t))\}_{t\in[0,1]} \), and, similarly, by (8.7), \( \text{sf}(\{A_n(t)\}_{t=-\infty}^\infty) = \text{sf}(\{g(S_n(t))\}_{t\in[0,1]} \). Recall that \( S(0) = S_n(0) = A_- \), \( S(1) = A_+ \) and \( S_n(1) = A_{+,n} \) (see (8.4) and (8.5)). We form the following loop
\[
(8.15) \quad g(A_-) \longrightarrow g(A_+) \longrightarrow g(A_{+,n}) \longrightarrow g(A_-),
\]
where the operators \( g(A_+) \) and \( g(A_{+,n}) \) are joined by the straight line \( L \). We claim that this loop is contractible, and therefore there is no spectral flow around this loop. To this end, it is sufficient to show that all operators in the loop are compact perturbations of a fixed operator, say, \( g(A_-) \).

Firstly, we show that the difference \( g(A(t)) - g(A_-) \) is compact for all \( -\infty \leq t \leq \infty \). By Lemma 2.21 we have
\[
(8.16) \quad g(A(t)) - g(A_-) = T^{A(t),A_-}_\phi \left( (A(t)^2 + 1)^{-1/4} (A(t) - A_-) (A^2_- + 1)^{-1/4} \right),
\]
with the double operator integral \( T^{A(t),A_-}_\phi \in \mathcal{B}(L_p(\mathcal{H})) \), \( p \geq 1 \). Hence, by equality (8.16) it is sufficient to show that \( (A(t)^2 + 1)^{-1/4} (A(t) - A_-) (A^2_- + 1)^{-1/4} \in \mathcal{L}_p(\mathcal{H}) \) for some \( p \geq 1 \).
We have
\[ (A(t)^2 + 1)^{-1/4}(A(t) - A_-)(A_-^2 + 1)^{-1/4} \]
\[ = -(A(t)^2 + 1)^{-1/4}(A_-^2 + 1)^{1/4} \times (A_-^2 + I)^{-1/4}B(t)(A_-^2 + 1)^{-1/4}. \]

Repeating the argument in [GLM+11] Remark 3.9 one can prove that the operator
\[ (A(t)^2 + 1)^{-1/4}(A_-^2 + I)^{1/4} \]
is bounded. Using the fact that
\[ B(t)(A_-^2 + 1)^{-1/2} \in \mathcal{L}_{p+1}(\mathcal{H}), \quad -\infty \leq t \leq \infty \]
(see [S.2] for \( t < \infty \) and [S.3] for \( t = \infty \)) and the three lines theorem (see also [GLM+11] Lemma 6.6), we infer that \( (A_-^2 + 1)^{-1/4}B(t)(A_-^2 + 1)^{-1/4} \in \mathcal{L}_{p+1}(\mathcal{H}), \) which implies that
\[ g(A(t)) - g(A_-) \in \mathcal{L}_{p+1}(\mathcal{H}), \quad -\infty \leq t \leq \infty. \]

Repeating the same argument, one can obtain that
\[ g(A_n(t)) - g(A_-) \in \mathcal{L}_{p+1}(\mathcal{H}), \quad -\infty \leq t \leq \infty. \]

Hence, the loop \( \{A(t)\}_{t \in [0,1]} \) consists of compact perturbations of the operator \( g(A_-) \), that is, it is contractible. Thus, there is no spectral flow around this loop, which means that
\[ \text{sf}\{g(S(t))\}_{t \in [0,1]} + \text{sf}\{g(A_+), g(A_{+,n})\} + \text{sf}\{g(S_n(t))\}_{t \in [1,0]} = 0. \]

Finally, by Lemma 8.8 we have \( \text{sf}\{g(A_+), g(A_{+,n})\} = 0 \) for sufficiently large \( n \in \mathbb{N} \). Hence, equality (8.17) implies that
\[ \text{sf}\{g(S(t))\}_{t \in [0,1]} = -\text{sf}\{g(S_n(t))\}_{t \in [1,0]} = \text{sf}\{g(S_n(t))\}_{t \in [0,1]}, \]
which completes the proof. \[ \square \]

Prior to proving the next result of this section, we recall that the spectral shift function \( \xi(\cdot; A_+, A_-) \) for the pair \( (A_+, A_-) \) is defined in [Theorem 7.1] and fixed via Theorem 7.2. In addition, the operators \( A_\pm \) are Fredholm, and therefore \( \xi(\cdot; A_+, A_-) \) is left and right-continuous at zero. In particular, 0 is a left and right Lebesgue point of \( \xi(\cdot; A_+, A_-) \). The result presented below generalises [ACS07] for operators with some essential spectra outside 0.

**Theorem 8.10.** Assume Hypothesis 8.1 then
\[ \frac{1}{2}(\xi(0+; A_+, A_-) + \xi(0--; A_+, A_-)) \]
\[ = \text{sf}\{A(t)\}_{t \rightarrow -\infty} - \frac{1}{2}[\dim(\ker(A_+)) - \dim(\ker(A_-))]. \]

**Proof.** By Proposition 8.7 we have
\[ \frac{1}{2}[(\xi(0+; A_{+,n}, A_-) + \xi(0--; A_{+,n}, A_-)) \]
\[ = \text{sf}\{A_{n}(t)\}_{t \rightarrow -\infty} - \frac{1}{2}[\dim(\ker(A_{+,n})) - \dim(\ker(A_-))]. \]

By Lemma 8.8 we have \( \dim(\ker(A_{+,n})) = \dim(\ker(A_+)) \) for sufficiently large \( n \in \mathbb{N} \). In addition, since \( A_\pm \) and \( A_{+,n} \) have discrete spectra at 0, the spectral shift functions \( \xi(\cdot; A_{+,n}, A_-) \) and \( \xi(\cdot; A_+, A_-) \) are step functions on a sufficiently small interval containing 0 (see e.g. [Yaf92, Proposition 8.2.8]). Hence, Corollary 7.2 implies...
that \( \xi(0_+; A_+, n, A_-) = \xi(0_+; A_+, A_-) \) and \( \xi(0_-; A_+, n, A_-) = \xi(0_-; A_+, A_-) \) for sufficiently large \( n \in \mathbb{N} \). Thus, for sufficiently large \( n \in \mathbb{N} \), we have

\[
\frac{1}{2} \left[ \xi(0_+; A_+, A_-) + \xi(0_-; A_+, A_-) \right] = \operatorname{sf}(\{ n \}_{t = -\infty}^\infty) - \frac{1}{2} \left[ \dim(\ker(A_+)) - \dim(\ker(A_-)) \right].
\]

(8.20)

Referring to Lemma \([8.9]\) we conclude that

\[
\frac{1}{2} \left[ \xi(0_+; A_+, A_-) + \xi(0_-; A_+, A_-) \right] = \operatorname{sf}(\{ A(t) \}_{t = -\infty}^\infty) - \frac{1}{2} \left[ \dim(\ker(A_+)) - \dim(\ker(A_-)) \right],
\]

as required.

\[ \square \]

**Remark 8.11.** We note that the assumptions (\( iv \)) and (\( v \)) of Hypothesis \([5.1]\) are not required for Theorem \([8.10]\).

As a corollary of Theorems \([7.8]\) and \([8.10]\) we obtain the following theorem, which is the main result of this section. This result is an extension of the Robin-Salamon theorem for those operators with some essential spectra outside 0 and without the assumption that the asymptotes \( A_\pm \) are boundedly invertible. As we will show in Section \([10]\) below our framework is suitable for differential operators on non-compact manifolds in any dimension.

**Theorem 8.12.** Assume Hypothesis \([8.1]\). Then the Witten index of the operator \( D_A \) exists and equals

\[
W_s (D_A) = \frac{1}{2} \left( \xi(0_+; A_+, A_-) + \xi(0_-; A_+, A_-) \right)
\]

(8.21)

\[
= \operatorname{sf}(\{ A(t) \}_{t = -\infty}^\infty) - \frac{1}{2} \left[ \dim(\ker(A_+)) - \dim(\ker(A_-)) \right].
\]

(8.22)

**Proof.** As we discussed above (see also \([8.8]\) Proposition 8.2.8), 0 is a left and right Lebesgue point of \( \xi(\cdot; A_+, A_-) \). Hence, by Theorem \([7.8]\) we have that the Witten index of the operator \( D_A \) exists and equals

\[
W_s (D_A) = \frac{1}{2} \left( \xi(0_+; A_+, A_-) + \xi(0_-; A_+, A_-) \right).
\]

On the other hand, Theorem \([8.10]\) implies \([8.22]\). \( \square \)

## 9. Generalised spectral flow

We continue to use the notation and assumptions of the previous section (see Hypothesis \([8.1]\)). As proved in Theorem \([8.12]\) the additional assumption that both asymptotes \( A_\pm \) are Fredholm, guarantees that the Witten index of the operator \( D_A \) exists and is equal, up to correction terms, to the spectral flow of the operators \( A(r) \) along the path \( \{ A(r) \}_{r \in \mathbb{R}} \), that is

\[
W_s (D_A) = \operatorname{sf}(\{ A(r) \}_{r \in \mathbb{R}}) - \frac{1}{2} \left[ \dim(\ker(A_+)) - \dim(\ker(A_-)) \right].
\]

(9.1)

When one removes the assumption that \( A_\pm \) are Fredholm operators the spectral flow along a path \( \{ A(t) \}_{t \in \mathbb{R}} \) is not defined. In this section we propose a suitable substitute for the spectral flow along the path \( \{ A(t) \}_{t \in \mathbb{R}} \) when the operators in the path are no longer Fredholm. In particular, we provide evidence
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for the statement made in [CGK16] that the principal trace formula provides a generalisation of spectral flow.

We recall (see Definition 7.4) that the Witten index

\[ W_s(D_A) = \lim_{t \to \infty} \text{tr}_N(e^{-tH_2} - e^{-tH_1}), \]

Furthermore, by the principal trace formula (see Theorem 6.4), we have that

\[ \text{tr}(e^{-tH_2} - e^{-tH_1}) = -\left(\frac{t}{\pi}\right)^{1/2} \int_0^1 \text{tr}(e^{-tA^2}(A_+ - A_-))ds, \]

where \( A_s = A_- + s(A_+ - A_-), \ s \in [0,1], \) is the straight line joining \( A_- \) and \( A_+. \)

Hence, assuming that the operators \( A_\pm \) are Fredholm, substitution of the previous two equalities into (9.1) implies that

\[ \lim_{t \to \infty} -\left(\frac{t}{\pi}\right)^{1/2} \int_0^1 \text{tr}(e^{-tA^2}(A_+ - A_-))ds = \text{sf}(A(r))_{r = -\infty}^{r = \infty} = \frac{1}{2} [\text{dim}(\ker(A_+)) - (\text{dim ker}(A_-))], \]

or equivalently,

\[ \text{sf}(A(r))_{r = -\infty}^{r = \infty} = \lim_{t \to \infty} -\left(\frac{t}{\pi}\right)^{1/2} \int_0^1 \text{tr}(e^{-tA^2}(A_+ - A_-))ds + \frac{1}{2} [\text{dim}(\ker(A_+)) - (\text{dim ker}(A_-))]. \]

The latter formula can be considered as a limit form of the integral formula of Theorem 8.3 for the spectral flow for a path of Fredholm operators \( \{A(r)\}_{r = -\infty}^{r = \infty} \) given by a \( p \)-relative trace class perturbation of a self-adjoint operator \( A_- \).

This is exactly the formula, which can be considered as generalised spectral flow. That is

**Definition 9.1.** Assume Hypothesis 5.1 and assume that the kernels of \( A_\pm \) are finite-dimensional. The generalised spectral flow \( \text{sf}_g(A(r))_{r = -\infty}^{r = \infty} \) of the path \( \{A(r)\}_{r = -\infty}^{r = \infty} \) is

\[ \text{sf}_g(A(r))_{r = -\infty}^{r = \infty} = \lim_{t \to \infty} -\left(\frac{t}{\pi}\right)^{1/2} \int_0^1 \text{tr}(e^{-tA^2}(A_+ - A_-))ds + \frac{1}{2} [\text{dim}(\ker(A_+)) - (\text{dim ker}(A_-))], \]

whenever the limit of the right-hand side exists.

**Remark 9.2.** Examples in low dimensions show that the limit can exist even if the operators \( A_\pm \) have continuous spectrum equal to the whole real line [CGG+16, CGLT16].

It is reasonable to ask what justifies this definition of ‘generalised spectral flow’. By analogy with the properties of spectral flow in the Fredholm case [Les05] we list the corresponding properties that follow from our definition of generalised spectral flow above.

(i) We have already shown above that if the operators \( A_\pm \) are Fredholm then generalised spectral flow reduces to the usual notion of spectral flow along paths of Fredholm operators.
(ii) It is obvious that this generalised spectral flow is additive on paths in the affine space of admissible perturbations by the properties of the integral on the right-hand side of (9.2).

(iii) Finally we need to have a certain path independence for this generalised spectral flow as long as paths remain in the appropriate affine space (a weak form of homotopy invariance).

This weak homotopy invariance property of generalised spectral flow needs a careful argument. It uses the fact that only $p$-relative trace-class perturbations of $A_-$ are permitted. We do this in Theorem 9.8 by proving that the functional

$$\alpha_A(X) = \text{tr}(e^{-tA^2}X), \quad A \in A_- + P(A_-), \quad X \in P(A_-),$$

where $P(A_-)$ stands for the space of $p$-relative trace class perturbation of $A_-$ gives an exact one form on the affine space $A_- + P(A_-)$.

We need to show that in the affine space of $p$-relative trace class perturbations, the functional $\alpha$ mentioned above is well defined. As before, $A_-$ is a self-adjoint operator and we let $B$ be a $p$-relative trace class perturbation of $A_-$. Since the function $u \mapsto e^{-u} (u + i)^{p+1}$, $t > 0$, is bounded, the $p$-relative trace-class assumption on the perturbation $B$ and Theorem 2.14 imply that for every $X \in P(A_-)$ the operator

$$e^{-tA^2}X = (D + i)^{p+1} e^{-tA^2} \left((A_+ + i)^{-p-1} - (A_- + i)^{-p-1}\right)X$$

$$+ (A_+ + i)^{p+1} e^{-tA^2} \cdot (A_- + i)^{-p-1}X$$

is a trace-class operator on $\mathcal{H}$. Therefore, the following definition makes sense.

**Definition 9.3.** Let $A_-$ be a self-adjoint operator on a complex separable Hilbert space $\mathcal{H}$ and let $p \in \mathbb{N}$ be fixed. Denote by $P(A_-)$ the vector space of all bounded self-adjoint operators $B$ on $\mathcal{H}$, which are $p$-relative trace-class operators with respect to $A_-$. Introduce the one form $\alpha$ on the affine space $A_- + P(A_-)$ defined at a point $A_+ \in A_- + P(A_-)$ by setting

$$\alpha_{A_+}(X) = \text{tr}(e^{-tA^2}X), \quad X \in P(A_-).$$

**Remark 9.4.** We note that Theorem 2.14 guarantees that if $B_1, B_2 \in P(A_-)$, then $B_2 \in P(A_- + B_1)$, since

$$B_2(A_- + B_1 + i)^{-p-1} = B_2(A_- + i)^{-p-1}$$

$$+ B_2\left((A_- + B_1 + i)^{-p-1} - (A_- + i)^{-p-1}\right) \in \mathcal{L}_1(\mathcal{H}).$$

Theorem 9.8 below, shows that the form $\alpha$ is exact by exhibiting a function $\theta$ on the affine space $A_- + P(A_-)$ such that

$$d\theta_{A_+}(X) = \alpha_{A_+}(X), \quad A_+ \in A_- + P(A_-), \quad X \in P(A_-).$$

We follow an argument similar to the one used in [ACS07], [CPS09].

Fix $B \in P(A_-)$ and denote by $A_s$, $s \in [0, 1]$, the straight line joining $A_-$ and $A_+$, that is

$$A_s = A_- + sB, \quad s \in [0, 1].$$
By Proposition 2.16 we can define the function $\theta$ on the affine space $A_- + P(A_-)$ by setting

$$\theta_{A_+} = \int_0^1 \text{tr}(Be^{-tA_2^2})ds,$$

where $A_+ = A_- + B \in A_- + P(A_-)$.

Before we proceed to the proof of Theorem 9.8, we establish some preliminary lemmas.

**Lemma 9.5.** Let $A_+ \in A_- + P(A_-)$ and $X \in P(A_-)$. We have

$$\lim_{r \to 0} \int_0^1 \text{tr}(Xe^{-t(A_+ + sriX)^2})ds = \int_0^1 \text{tr}(Xe^{-tA_2^2})ds.$$

**Proof.** The argument is similar to that in the proof of Lemma 2.17. By Theorem 2.14 (see also Remark 2.15) we have

$$\lim_{r \to 0} \text{tr}(Xe^{-t(A_+ + sriX)^2}) = 0.$$

Since, in addition, the family of functions $s \mapsto \|Xe^{-t(A_+ + sriX)^2}\|_1$ is uniformly bounded with respect to $r$ by a bounded function, the dominated convergence principle implies that

$$\lim_{r \to 0} \int_0^1 \text{tr}(Xe^{-t(A_+ + sriX)^2})ds = \int_0^1 \text{tr}(Xe^{-tA_2^2})ds. \quad \Box$$

**Lemma 9.6.** For every $j = 1, \ldots, p$, $z \in \mathbb{C} \setminus \mathbb{R}$ and $X \in P(A_-)$ we have

$$(A_{s_1} - z)^{-p+j-1}X(A_{s_2} - z)^{-j} \in L_1(\mathcal{H}), \quad s_1, s_2 \in [0, 1]$$

and

$$\left\|(A_{s_1} - z)^{-p+j-1}X(A_{s_2} - z)^{-j} - (A_{s_2} - z)^{-p+j-1}X(A_{s_2} - z)^{-j}\right\|_1 \to 0$$

as $s_2 - s_1 \to 0$.

**Proof.** We write

$$(A_{s_1} - z)^{-p+j-1}X(A_{s_2} - z)^{-j} = \left((A_{s_1} - z)^{-p+j-1} - (A_- - z)^{-p+j-1}\right)X \left((A_{s_2} - z)^{-j} - (A_- - z)^{-j}\right)$$

$$+ (A_- - z)^{-p+j-1}X \left((A_{s_2} - z)^{-j} - (A_- - z)^{-j}\right)$$

$$+ (A_{s_1} - z)^{-p+j-1}X \left((A_{s_2} - z)^{-j} - (A_- - z)^{-j}\right) \cdot X(A_- - z)^{-j}$$

$$- (A_- - z)^{-p+j-1}X(A_- - z)^{-j}.$$

Hence, the claim follows from Theorem 2.14. \quad \Box

Let $f(x) = e^{-tx^2}$, $x \in \mathbb{R}$, $t > 0$ and let $T^{A_s, A_j}_{f, a_k}$ be the double operator integral as in Proposition 2.18.
Lemma 9.7. For the derivative $\| \cdot \|_1 \frac{d}{ds} e^{-tA_s^2}$ of the family function $s \mapsto e^{-tA_s^2}$, $s \in [0,1]$, taken in the trace-class norm we have

$$\| \cdot \|_1 \frac{d}{ds} e^{-tA_s^2} = \sum_{k=1,2} T_{f,a_k} \left( \sum_{j=1}^{p_0} (A_s - ia_k)^{-p_0+j-1} B(A_s - ia_k)^{-j} \right) \in \mathcal{L}_1(\mathcal{H}).$$

Proof. Let $p_0 = 2 \left[ \frac{p}{2} \right] + 1$. By the definition of $\| \cdot \|_1 \frac{d}{ds} e^{-tA_s^2}$ and the double operator integrals $T_{f,a_k}^{A_s}$, we have

$$\| \cdot \|_1 \frac{d}{ds} e^{-tA_s^2} = \| \cdot \|_1 \lim_{s_1 \to s} \frac{e^{-tA_{s_1}^2} - e^{-tA_s^2}}{s_1 - s}$$

$$= \| \cdot \|_1 \lim_{s_1 \to s} \sum_{k=1,2} T_{f,a_k} \left( (A_{s_1} + ia_k)^{-p_0} - (A_s + ia_k)^{-p_0} \right)$$

$$= \| \cdot \|_1 \lim_{s_1 \to s} \sum_{k=1,2} T_{f,a_k} \left( \sum_{j=1}^{p_0} (A_{s_1} + ia_k)^{-p_0+j-1} (A_s - A_{s_1})(A_s + ia_k)^{-j} \right)$$

$$= \| \cdot \|_1 \lim_{s_1 \to s} \sum_{k=1,2} T_{f,a_k}^{A_{s_1}} \left( \sum_{j=1}^{p_0} (A_{s_1} + ia_k)^{-p_0+j-1} B(A_s + ia_k)^{-j} \right)$$

By Lemma 9.6 we have

$$(A_{s_1} + ia_k)^{-p_0+j-1} B(A_s + ia_k)^{-j}$$

converges to

$$(A_s + ia_k)^{-p_0+j-1} B(A_s + ia_k)^{-j}$$

in $\mathcal{L}_1(\mathcal{H})$ as $s_1 \to s$. By Remark 2.15 and Theorem 2.4, we infer that

$$T_{f,a_k}^{A_{s_1}} \to T_{f,a_k}^{A_s}, \quad s_1 \to s$$

pointwise on $\mathcal{L}_1(\mathcal{H})$. Hence,

$$\| \cdot \|_1 \frac{d}{ds} e^{-tA_s^2} = \sum_{k=1,2} T_{f,a_k}^{A_s} \left( \sum_{j=1}^{p_0} (A_s + ia_k)^{-p_0+j-1} B(A_s + ia_k)^{-j} \right) \in \mathcal{L}_1(\mathcal{H}),$$

as required. \qed

The next theorem is the main result of the present section. It shows that the one form $\alpha$ defined in Definition 9.3 is exact, which implies that the right-hand side of equality 11.2 does not depend on the $C^1$-path joining the endpoints $A_-$ and $A_+$. This provides the strongest evidence for regarding (11.2) as a generalisation of spectral flow for paths not necessarily consisting of Fredholm operators. The proof of Theorem 9.8 uses ideas from ACS07, CPS09 and the approximation technique employed in the previous sections.

Theorem 9.8. For every $X \in P(A_-)$ we have, for the exterior derivative:

$$d\theta_{A_+}(X) = \alpha_{A_+}(X).$$

That is, the one form $\alpha$ is exact.
Proof. Fix $X \in \mathcal{P}(A_-)$ and let $B = A_+ - A_-$. By definition,
\[
d\theta_{A_+}(X) = \frac{d}{dr} \bigg|_{r=0} \theta_{A_+ + rX}
\]
(9.4) \hspace{1cm} \lim_{r \to 0} \frac{1}{r} \int_0^1 \text{tr} \left( (A_+ + rX - A_-) e^{-t(A_+ + srX)^2} - (A_+ - A_-) e^{-tA_-^2} \right) ds
\]
\[
= \lim_{r \to 0} \int_0^1 \text{tr}(X e^{-t(A_+ - srX)^2}) ds + \lim_{r \to 0} \frac{1}{r} \int_0^1 \text{tr} \left( B(e^{-t(A_+ + srX)^2} - e^{-tA_-^2}) \right) ds
\]

Now apply Lemma 9.5 to see that
(9.5) \hspace{1cm} \lim_{r \to 0} \int_0^1 \text{tr}(X e^{-t(A_+ - srX)^2}) ds = \int_0^1 \text{tr}(X e^{-tA_-^2}) ds.

For the second term on the right hand side of (9.4) (in a fashion similar to\cite{CPS09} (Eq. (6))), we claim that
(9.6) \hspace{1cm} \lim_{r \to 0} \int_0^1 \text{tr} \left( B \frac{1}{r}(e^{-t(A_+ + srX)^2} - e^{-tA_-^2}) \right) ds = \text{tr}(X e^{-tA_-^2}) - \int_0^1 \text{tr}(X e^{-tA_-^2}) ds.

Let, as before, $f(x) = e^{-tx^2}$, $x \in \mathbb{R}$ and $p_0 = 2\lfloor \frac{p}{2} \rfloor + 1$. With the double operator integrals as in Proposition 2.3 we have
\[
\frac{1}{r}B \left( e^{-t(A_+ + srX)^2} - e^{-tA_-^2} \right)
\]
\[
= \frac{1}{r}B \sum_{k=1,2} T_{f,ak}^{A_+,srX,A_-} \left( (A_s + srX - ia_k)^{-p_0} - (A_s - ia_k)^{-p_0} \right)
\]
\[
= \frac{1}{r}B \sum_{k=1,2} T_{f,ak}^{A_+,srX,A_-} \left( \sum_{j=1}^{p_0} (A_s + srX - ia_k)^{-p_0+j-1} \cdot srX(A_s - ia_k)^{-j} \right)
\]
\[
= sB \sum_{k=1,2} T_{f,ak}^{A_+,srX,A_-} \left( \sum_{j=1}^{p_0} (A_s + srX - ia_k)^{-p_0+j-1} \cdot X(A_s - ia_k)^{-j} \right).
\]

Using again the convergence
\[
\lim_{r \to 0} \left\| (A_s + srX - ia_k)^{-p_0+j-1} \cdot X(A_s - ia_k)^{-j} - (A_s - ia_k)^{-p_0+j-1} \cdot X(A_s - ia_k)^{-j} \right\|_1 = 0
\]
and continuity of double operators integrals $T_{f,ak}^{A_+,srX,A_-}$ (see Theorem 2.4) we obtain that
\[
\lim_{r \to 0} \text{tr} \left( B \frac{1}{r}(e^{-t(A_+ + srX)^2} - e^{-tA_-^2}) \right)
\]
\[
= s \text{tr} \left( B \sum_{k=1,2} T_{f,ak}^{A_+,A_-} \left( \sum_{j=1}^{p_0} (A_s - ia_k)^{-p_0+j-1} \cdot X(A_s - ia_k)^{-j} \right) \right).
\]

We set
(9.7) \hspace{1cm} B_n = \chi_{[-n,n]}(A_s)B_X\chi_{[-n,n]}(A_s), \hspace{0.5cm} X_n = \chi_{[-n,n]}(A_s)X\chi_{[-n,n]}(A_s), \hspace{0.5cm} n \in \mathbb{N}.

As $B, X \in \mathcal{P}(A_s)$, we have $B_n, X_n \in \mathcal{L}_1(\mathcal{H})$ for any $n \in \mathbb{N}$ (see\cite{2132}). Moreover, Lemma 2.9 combined with Lemma 9.6 implies that \{(A_s - ia_k)^{-p_0+j-1} \cdot X(A_s - ia_k)^{-j}\}_{n \in \mathbb{N}} converges to $(A_s - ia_k)^{-p_0+j-1} \cdot X(A_s - ia_k)^{-j}$ and \{(A_s - ia_k)^{-p_0+j-1} \cdot B(X(A_s - ia_k)^{-j})\}_{n \in \mathbb{N}} converges to $(A_s - ia_k)^{-p_0+j-1} \cdot B(A_s - ia_k)^{-j}$ in $\mathcal{L}_1(\mathcal{H})$. 

Hence,
\[
\lim_{r \to 0} \text{tr} \left( B \frac{1}{r} (e^{-t(A_x + srX)^2} - e^{-tA^2_x}) \right) = \lim_{n \to \infty} s \text{tr} \left( B_0 \sum_{i=1,2} T_{f,a_i}^{A_x, A_x} \left( \sum_{m} (A_s - ia_k)^{-p_0} X_n(A_s - ia_k)^{-m+p_0} \right) \right)
\]
\[
= \lim_{n \to \infty} s \sum_{i=1,2} \sum_{m} \text{tr} \left( B_0 (A_s - ia_k)^{-m+p_0} T_{f,a_i}^{A_x, A_x} (X_n)(A_s - ia_k)^{-m+p_0} \right)
\]
\[
= \lim_{n \to \infty} s \sum_{i=1,2} \sum_{m} \text{tr} \left( T_{f,a_i}^{A_x, A_x} \left( (A_s - ia_k)^{-m+p_0} B(A_s - ia_k)^{-p_0} X_n \right) \right),
\]
where the last equality follows the definition of the double operators integrals on \( \mathcal{B}(\mathcal{H}) \) via duality (see e.g. [BS03]). Therefore,
\[
\lim_{r \to 0} \text{tr} \left( B \frac{1}{r} (e^{-t(A_x + srX)^2} - e^{-tA^2_x}) \right) = \lim_{n \to \infty} s \sum_{i=1,2} \sum_{m} \text{tr} \left( T_{f,a_i}^{A_x, A_x} \left( (A_s - ia_k)^{-m+p_0} B(A_s - ia_k)^{-p_0} X \right) \right).
\]

By Lemma 9.7 we obtain that
\[
\lim_{r \to 0} \text{tr} \left( B \frac{1}{r} (e^{-t(A_x + srX)^2} - e^{-tA^2_x}) \right) = s \text{tr} \left( X \frac{d}{ds} e^{-tA^2_x} \right).
\]

Therefore,
\[
\lim_{r \to 0} \int_0^1 \text{tr} \left( B \frac{1}{r} (e^{-t(A_x + srX)^2} - e^{-tA^2_x}) \right) ds = \int_0^1 s \text{tr} \left( X \frac{d}{ds} e^{-tA^2_x} \right) ds.
\]

Integrating by parts the latter equality (see also [CPS09 last display on page 1820]) we obtain that
\[
\int_0^1 s \text{tr} \left( X \frac{d}{ds} e^{-tA^2_x} \right) ds = \text{tr} \left( X e^{-tA^2_x} \right) - \int_0^1 \text{tr} \left( X e^{-tA^2_x} \right) ds,
\]
and therefore, 9.6 is proved. Thus,
\[
\frac{d\theta_{A_+}(X)}{ds} = \int_0^1 \text{tr} (X e^{-tA^2_x} ds + \text{tr} (X e^{-tA^2_x} - \int_0^1 \text{tr} (X e^{-tA^2_x} ds
\]
\[
= \alpha_{A_+}(X),
\]
as required. \( \square \)

Remark 9.9. In this article we have not attempted to discuss what happens when we work with Phillips’ spectral flow for paths in a semi-finite von Neumann algebra. In fact much of what we have discussed here goes through without significant change. The definition of generalised spectral flow also certainly carries over. Further study of examples from condensed matter theory is required in order to appreciate whether the semi-finite case might be of interest. \( \diamond \)
10. Example of the Dirac operator in $\mathbb{R}^d$

In this section we supplement the abstract discussion by an example for which our general assumption holds and hence the results of Sections 7, 8 are applicable. Our primary example, the multidimensional Dirac operator and its perturbations given by multiplication operators by matrix valued functions, satisfy Hypothesis 5.1. Thus, our framework is indeed suitable for differential operators on certain non-compact manifolds.

10.1. Setting. Throughout this section we fix $d \in \mathbb{N}$. For each $k = 1, \ldots, d$, we denote by $\partial_k$ the operators of partial differentiation, that is operators in $L^2(\mathbb{R}^d)$ defined as

$$\partial_k = -i \frac{\partial}{\partial t_k}.$$ 

We denote the tuple $(\partial_1, \ldots, \partial_d)$ by $\nabla$.

Let $n(d) = 2^{d+1}$. Let $\gamma_k \in M_{n(d)}(\mathbb{C})$, $0 \leq k \leq d$, be Clifford algebra generators, that is,

(i) $\gamma_k \gamma_k^* = 1$ for $0 \leq k \leq d$.

(ii) $\gamma_k \gamma_{k'} = -\gamma_{k'} \gamma_k$ for $0 \leq k_1, k_2 \leq d$, such that $k_1 \neq k_2$.

We use the notation $\gamma = (\gamma_1, \ldots, \gamma_d)$.

Definition 10.1. Let $m \geq 0$. Define the Dirac operator as an unbounded operator $D$ acting in the Hilbert space $\mathbb{C}^n(d) \otimes L^2(\mathbb{R}^d)$ with domain $\text{dom}(D) = \mathbb{C}^n(d) \otimes W^{1,2}(\mathbb{R}^d)$ by the formula

$$(10.1) \quad D = \gamma \cdot \nabla + m\gamma_0.$$ 

It is well-known that the operator $D$ is self-adjoint. Furthermore,

$$D^2 = -\Delta + m^2,$$

where $-\Delta = -\sum_{k=1}^d \frac{\partial^2}{\partial x_k^2}$ is the Laplace operator.

Suppose that $V = \{\phi_{ij}\}_{i,j=1}^{n(d)}$ is a hermitian matrix of functions, such that $\phi_{ij} \in L^\infty(\mathbb{R}^d)$. We also write $V$ for the bounded operator of multiplication by this matrix function $V$ on the Hilbert space $\mathbb{C}^n(d) \otimes L^2(\mathbb{R}^d)$. We also identify a function $f \in L^\infty(\mathbb{R}^d)$ with the operator on $L^2(\mathbb{R}^d)$ of multiplication by $f$.

For the example of the current section we set

$$A_- = D, \quad B_+ = V$$

and

$$B(t) = \theta(t)B_+,$$

where $\theta$ satisfies [5.4].

10.2. Verification of Hypothesis 5.1. Recall (see [BS77] and [Sim03]) that the space $l_1(L_2)(\mathbb{R}^d)$ is defined as

$$l_1(L_2)(\mathbb{R}^d) := \left\{ f \in L^0(\mathbb{R}^d) : \sum_{n \in \mathbb{Z}^d} \| f\chi_{Q+n} \|_2 < \infty \right\},$$

where $Q$ denotes the unit cube in $\mathbb{R}^d$ centered at 0. The space $l_1(L_2)(\mathbb{R}^d)$ is equipped with the norm defined by

$$\| f \|_{l_1(L_2)(\mathbb{R}^d)} := \sum_{n \in \mathbb{Z}^d} \| f\chi_{Q+n} \|_2, \quad f \in l_1(L_2)(\mathbb{R}^d).$$
Proposition 10.2. Assume that \( V = \{ \phi_{ij} \}_{i,j=1}^{n(d)} \) is such that \( \phi_{ij} \in l_1(L^2(\mathbb{R}^d)) \). Then \( V \) is a \( d \)-relative trace-class perturbation with respect to \( \mathcal{D} \), that is Hypothesis (ii) is satisfied.

Proof. Since \( \phi_{ij} \in l_1(L^2(\mathbb{R}^d)) \), Theorem 4.4 implies that the matrix elements \( \phi_{ij}(-\Delta + 1)^{-d+1} \) are trace class operators (on \( L^2(\mathbb{R}^d) \)) for all \( 1 \leq i, j \leq n(d) \). Hence, the operator

\[
V(D^2 + 1)^{-\frac{d-1}{2}} = (\phi_{ij}(-\Delta + 1)^{-\frac{d-1}{2}})_{i,j=1}^{n(d)}
\]

is a trace class operator (on \( \mathbb{C}^{n(d)} \otimes L^2(\mathbb{R}^d) \)). Therefore, \( V(D + i)^{-1 - d} \in \mathcal{L}_1(\mathbb{C}^{n(d)} \otimes L^2(\mathbb{R}^d)) \). \( \Box \)

Our next task is to establish a sufficient condition on the matrix \( V \) for Hypothesis (iii) to hold. Since \( D^2 = -\Delta + m^2 \), we have that

\[
[D^2, V] = \left( [-\Delta, \phi_{ij}] \right)_{i,j=1}^{n(d)},
\]

whenever the commutators \([-\Delta, \phi_{ij}]\) are well-defined. Therefore, introducing \( L^k_{-\Delta}, j \in \mathbb{N} \), as in (5.6) (with \( A^2 = -\Delta \)), we obtain that \( V \in \text{dom}(L^k_{-\Delta}) \) for some \( k \in \mathbb{N} \), provided that \( \phi_{ij} \in \text{dom}(L^k_{-\Delta}) \) for any \( i, j = 1, \ldots, n(d) \). In this case,

\[
(10.2) \quad L^k_{D^2}(V) = (1 + D^2)^{-k/2}[D^2, T]^{(k)} = \left( L^k_{-\Delta + m^2}(\phi_{ij}) \right)_{i,j=1}^{n(d)}.
\]

Proposition 10.3. Let \( k \in \mathbb{N} \) be fixed. Assume that \( \phi \in W^{2k, \infty}(\mathbb{R}^n) \). Then \( \phi \in \bigcap_{j=1}^{2k} \text{dom}(L^j_{-\Delta + m^2}) \).

Proof. Let \( k \in \mathbb{N} \) be fixed. Since \( \phi \in W^{2k, \infty}(\mathbb{R}^n) \), we have that \( (\Delta)^j(\phi \xi) \in L^2(\mathbb{R}^n) \) for every \( \xi \in \text{dom}(\Delta)^j \), \( j = 1, \ldots, k \). That is \( \phi \text{dom}(\Delta)^j \subset \text{dom}(\Delta)^j \) for all \( j = 1, \ldots, 2k \).

Recall that \( \partial_k = \frac{\partial}{\partial x_k} \) and if \( \phi \in L^\infty(\mathbb{R}^d) \) with \( \frac{\partial \phi}{\partial x_k} \in L^\infty(\mathbb{R}^d) \), \( k = 1, \ldots, d \), then \( \phi \text{dom}(\partial_k) \subset \text{dom}(\partial_k) \) and for all \( \xi \in \text{dom}(\partial_k) \) we have

\[
(10.3) \quad [\partial_k, \phi]\xi = \frac{1}{i} \frac{\partial \phi}{\partial x_k} \xi, \quad k = 1, \ldots, d.
\]

By (10.3) we have

\[
[\Delta, \phi] = \sum_{j=1}^{n} [\partial_j^2 \phi, \phi] = \sum_{j=1}^{n} \partial_j [\partial_j \phi, \phi] + \sum_{j=1}^{n} [\partial_j \phi, \partial_j \phi] = \frac{1}{i} \sum_{j=1}^{n} \left( \partial_j \frac{\partial \phi}{\partial x_j} + \frac{\partial \phi}{\partial x_j} \partial_j \right) = \frac{1}{i} \sum_{j=1}^{n} \left( 2 \partial_j \frac{\partial \phi}{\partial x_j} - [\partial_j, \frac{\partial \phi}{\partial x_j}] \right)
\]

\[
= \frac{2}{i} \sum_{j=1}^{n} \partial_j \frac{\partial \phi}{\partial x_j} + \sum_{j, \ell=1}^{n} \frac{\partial^2 \phi}{\partial x_j \partial x_{\ell}},
\]
Therefore,
\[
(1 + m^2 - \Delta)^{-1/2}[\Delta, \phi] = \frac{2}{\ell} \sum_{j=1}^{n} \partial_j (1 + m^2 - \Delta)^{-1/2} \frac{\partial \phi}{\partial x_j} + \sum_{j, \ell=1}^{n} (1 + m^2 - \Delta)^{-1/2} \frac{\partial^2 \phi}{\partial x_j \partial x_\ell}.
\]

Since \( \phi \in W^{2k, \infty}(\mathbb{R}^n) \), it follows that the operators \( \frac{\partial^2 \phi}{\partial x_j \partial x_\ell} \) and \( M_{\phi, j, \ell} \), \( j, \ell = 1, \ldots, n \), are bounded. Since the operator \( \partial_j (1 + m^2 - \Delta)^{-1/2} \) is also bounded, we infer that
\[
(1 + m^2 - \Delta)^{-1/2}[\Delta, \phi] \in B(L^2(\mathbb{R}^n)).
\]

Continuing this process, we obtain that
\[
(10.4) \quad (1 - \Delta)^{-j}[\Delta, \phi] \in B(L^2(\mathbb{R}^n)), \quad j = 1, \ldots, k,
\]
that is \( \phi \in \bigcap_{j=1}^{2k} \text{dom}(L^2_{-\Delta}) \).

Combining now Propositions 10.2 and 10.3 we arrive at the following

**Theorem 10.4.** Let \( A_- = \mathcal{D} \) be the Dirac operator on \( C^{n(d)} \otimes L^2(\mathbb{R}^d) \) defined by (10.1), \( d \in \mathbb{N} \). Assume that \( V = \{ \phi_{ij} \}_{i,j=1}^{n(d)} \) is such that
\[
\phi_{ij} \in l_1(L^2(\mathbb{R}^d)) \cap W^{4p, \infty}(\mathbb{R}^d), \quad i, j = 1, \ldots, n(d).
\]
Then the operator \( A_- = \mathcal{D}(d) \) and the perturbation \( B_+ = V \) satisfy Hypothesis 5.5 (and hence also Hypothesis 5.1) with \( p = d \).

10.3. **The index of \( D_A \).** Everywhere below we assume that the perturbation \( V = \{ \phi_{ij} \}_{i,j=1}^{n(d)} \) satisfies the assumption of Theorem 10.4.

Since \( \mathcal{D}^2 = -\Delta + m^2 \), it follows that the operator \( \mathcal{D} \) has purely absolutely continuous spectrum, which coincides with \((-\infty - m) \cup [m, \infty)\). In the case, when \( m \) is strictly positive, the assumption that the operator \( V(\mathcal{D} + i)^{-d-1} \) is compact together with Weyl’s theorem guarantees that the operator \( \mathcal{D} + V \) has purely discrete spectrum in the interval \((-m, m)\). In particular, if \( \mathcal{D} + V \) is also invertible, then by Theorem 5.3 the corresponding operator
\[
D_A = \frac{d}{dt} \otimes 1 + 1 \otimes \mathcal{D} + \theta V,
\]
(see (5.16)) is Fredholm. Furthermore, since in this case the spectral shift function \( \xi(\cdot; \mathcal{D}+V, \mathcal{D}) \) for the pair \( (\mathcal{D}+V, \mathcal{D}) \) is constant in a neighbourhood of zero Theorem 7.8 implies that
\[
\text{index}(D_A) = \xi(0; \mathcal{D}+V, \mathcal{D}).
\]

If the operator \( \mathcal{D}+V \) is not invertible, then the operator \( D_A \) is no longer Fredholm. However, since in this case the spectral shift function \( \xi(\cdot; \mathcal{D}+V, \mathcal{D}) \) is left and right continuous at zero, it follows that 0 is, in particular, left and right Lebesgue point of \( \xi(\cdot; \mathcal{D}+V, \mathcal{D}) \). Hence, Theorem 7.8 again implies that
\[
W_\ast(D_A) = \frac{1}{2} [\xi(0+; \mathcal{D}+V, \mathcal{D}) + \xi(0-; \mathcal{D}+V, \mathcal{D})].
\]
In particular, if \( d = 3 \) and the potential \( V \) is a magnetic potential, that is
\[
V = \sum_{n=1}^{3} \gamma_j A_j, \quad A_j \in L_3(\mathbb{R}^3) \cap L_1(\mathbb{R}^3),
\]
then \cite[Section 5.1]{Sa01} implies that \( \xi(0; D + V, D) = 0 \), and therefore, by (10.3) we obtain that
\[
W_s(D_A) = 0.
\]

Our main interest lies in the massless Dirac operator, where \( m = 0 \). In this case, the spectrum of \( D \) covers the whole real line, and therefore, whatever the potential \( V \), the operator \( D_A \) in (10.5) is never Fredholm. However, Theorem [10.4] guarantees that the pair
\[
A_+ = D, \quad B_+ = V,
\]
both satisfy Hypothesis [5.1] and therefore, by Theorem [8.12] to study whether the Witten index of \( D_A \) exists in this case it is sufficient to study the spectral shift function \( \xi(\cdot; D + V, D) \) for the pair \( (D + V, D) \) and its behaviour near zero.

Although the spectral shift function for the second order operators is well studied, there is a sparse literature available for the spectral shift function for the first order operators \( D \) and \( D + V \) (see e.g. \cite{Sa01, TdA11, BR99}). Furthermore, the majority of papers on this topic study the massive case, \( m > 0 \), and are, therefore, not applicable to our case. Our initial investigation, in collaboration with F. Gesztesy and R. Nichols, shows that for a sufficiently good perturbation \( V \), the spectral shift function \( \xi(\cdot; D + V, D) \) is left and right continuous at zero even in the massless case. Hence, the Witten index of the operator \( D_A \) exists and
\[
W_s(D_A) = \xi(0; D + V, D).
\]

However, the proof of left/right continuity of the spectral shift function \( \xi(\cdot; D + V, D) \) at zero involves a generalisation of the original formula for the spectral shift function due to Krein (see \cite{Yaf92}) in terms of a perturbation determinant as well as to an extensive analysis of the spectrum of the perturbed operator \( D + V \). The full details of this approach as well as the exact statement of continuity of \( \xi(\cdot; D + V, D) \) involve lengthy arguments and we defer the discussion to a separate manuscript \cite{CGL+18} that is in preparation.

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