Spectral Theory of Boundary Value Problems
for Dirac Type Operators

Jochen Brüning and Matthias Lesch

ABSTRACT. The purpose of this Note is to describe a unified approach to the fundamental results in the spectral theory of boundary value problems, restricted to the case of Dirac type operators. Even though many facts are known and well presented in the literature (cf. the monograph of Booss-Wojciechowski [7]), we simplify and extend or sharpen most results by using systematically the simple structure which Dirac type operators display near the boundary. Thus our approach is basically functional analytic, and consequently we achieve results which apply to more general situations than compact manifolds with boundary.

1. The compact case

Let $\widetilde{M}$ be a compact oriented Riemannian manifold of dimension m, $\widetilde{E} \to \widetilde{M}$ a hermitian vector bundle, and $\widetilde{D}$ a symmetric elliptic differential operator of order $d \in \mathbb{Z}_+$ on $C^\infty(\widetilde{E})$. The classical results on existence, uniqueness, and regularity of solutions of $\widetilde{D}$ are among the cornerstones of Global Analysis:

- $\widetilde{D}$ is essentially self-adjoint in $L^2(\widetilde{E})$ with domain $C^\infty(\widetilde{E})$ (by slight abuse of notation, we denote the closure of $\widetilde{D}$ by the same symbol); $\quad$ (1.1)

- $\widetilde{D}$ is a Fredholm operator (of index 0), i.e. there are a bounded operator $\widetilde{Q}$ and compact operators $\widetilde{K}_r, \widetilde{K}_l$ in $L^2(\widetilde{E})$ such that $\quad$ (1.2)

$$\widetilde{D}\widetilde{Q} = I - \widetilde{K}_r, \qquad \widetilde{Q}\widetilde{D} = I - \widetilde{K}_l;$$

- with respect to the Sobolev scale $H_s(\widetilde{E}) := \mathcal{D}((\widetilde{D}^2 + I)^{s/2d})$, $s \geq 0$, $\widetilde{Q}$ is of order $-d$ and $\widetilde{K}_{r/l}$ of order $-\infty$. $\quad$ (1.3)

The restriction to symmetric operators is not essential since we may always consider a given elliptic operator together with its adjoint. But it is a technical advantage for more refined questions like index theorems: We bring in an isometric

involution $\widetilde{\omega}$ on $\widetilde{E}$ which anticommutes with $\widetilde{D}$ on $C^\infty(\widetilde{E})$ and hence produces a splitting

$$(1.4) \qquad \widetilde{D} = \begin{pmatrix} 0 & \widetilde{D}_- \\ \widetilde{D}_+ & 0 \end{pmatrix} \quad \text{on} \quad C^\infty(\widetilde{E}_+) \oplus C^\infty(\widetilde{E}_-),$$

with $\widetilde{E}_\pm$ the ± 1–eigenbundle of $\widetilde{\omega}$. Then, by the well–known formula of McKean-Singer we have

$$(1.5) \qquad \text{ind}\,\widetilde{D}_+ = \text{tr}\big[\widetilde{\omega} e^{-t\widetilde{D}^2}\big], \quad t > 0.$$

It is hence of great importance that (cf. eg. [**12**, Lemma 1.9.1])

- for any differential operator $\widetilde{P}$ of order p on $C^\infty(\widetilde{E})$, we have an asymptotic expansion

$$(1.6) \qquad \text{tr}\Big[\widetilde{P} e^{-t\widetilde{D}^2}\Big] \sim_{t \to 0+} \sum a_j(\widetilde{D}, \widetilde{P}) t^{(j-m-p)/d}.$$

Even though it took a long time after the original proof of the Atiyah–Singer Index Theorem [**2**], [**15**] until a complete proof could be based on (1.4) and (1.5) (cf. [**3**], [**11**]), the heat equation method now seems to be the most powerful tool for extensions of the Index Theorem. Recall that for the important class of twisted Dirac operators, with $\widetilde{E} = \widetilde{S} \otimes \widetilde{F}, \widetilde{S}$ a spin bundle on $\widetilde{M}$, this theorem reads

- $\text{ind}\,\widetilde{D}_+ = \displaystyle\int_{\widetilde{M}} \hat{A}(\widetilde{M}) \wedge \text{ch}\,\widetilde{F}.$ $\hfill (1.7)$

2. Compact manifolds with boundary

We want to present the extension of the main results quoted above ((1.1), (1.2), (1.3), (1.6), (1.7)) to Dirac type operators on manifolds with boundary. Though a good part of our results is more or less known, we obtain a conceptually as well as technically transparent derivation of this theory, with considerable simplifications and extensions in most cases. Moreover, the functional analytic approach we have developed lends itself naturally to substantial generalizations, e.g. to situations with non-compact boundaries.

To explain our work in greater detail, we consider a compact hypersurface, N, in $\widetilde{M}$ which bounds an open subset, M, of $\widetilde{M}$. We assume that N is oriented as the boundary of M. Then we put $E := \widetilde{E} \upharpoonright M$, $D := \widetilde{D} \upharpoonright C^\infty(\overline{M})$. Then D is a first order elliptic differential operator on M, and symmetric in $L^2(E)$ with domain $C_0^\infty(E)$. If D is of *Dirac type* (in the sense of [**12**, Chap. 4, 4.4]) we then obtain in a tubular neighbourhood, U, of N in $\widetilde{M}$ a very simple separation of variables. In fact, U is isometric to $(-\varepsilon_0, \varepsilon_0) \times N$ with metric $dx^2 \oplus g_N(x), x \in (-\varepsilon_0, \varepsilon_0)$, g_N a smooth family of metrics on N, and with $E_N := \widetilde{E} \upharpoonright N$ we obtain the following result.

LEMMA 2.1. *Let D be of Dirac type. As operator in $L^2(E \upharpoonright U)$ with domain $C_0^\infty(E \upharpoonright U)$, D is unitarily equivalent to an operator of the form*

$$(2.1) \qquad \gamma\left(\frac{d}{dx} + A(x)\right)$$

in $L^2((-\varepsilon_0, \varepsilon_0), L^2(E_N))$ with domain $C_0^\infty((-\varepsilon_0, \varepsilon_0), C^\infty(E_N))$, where $\gamma \in \mathcal{L}(L^2(E_N))$ and $A(x)$ is (the closure of) a symmetric elliptic differential operator on E_N of first order; $\mathcal{D}(A(x)) =: \mathcal{D}$ is independent of x and $A(x)$ depends smoothly on $x \in (-\varepsilon_0, \varepsilon_0)$.

Moreover, the following relations hold:

(2.2a) $\qquad \gamma^* = -\gamma, \quad \gamma^2 = -I,$

(2.2b) $\qquad \gamma(\mathcal{D}) = \mathcal{D} \text{ and } \gamma A(x) + A(x)\gamma = 0, \quad x \in (-\varepsilon_0, \varepsilon_0).$

This lemma has been widely used for some time, especially in the product case $(g_N(x) \equiv g_N(0))$ where it plays a prominent role in [4]. For non-product metrics some care is needed to compute $A(x)$ in each specific case, cf. e.g. [12, Sec. 3.10] and [8, Sec. 5].

We will base our analysis on a thorough study of the operator equation (2.1) with the structure properties (2.2); *these properties will be assumed throughout this paper*. This is reasonable since the results we are aiming at can be obtained from merging "interior analysis" (to be carried out on $\widetilde{M}$) with "boundary" analysis involving the operator (2.1).

The main difference between the analysis of D and $\widetilde{D}$ lies, of course, in the fact that D is not essentially self-adjoint on $C_0^\infty(E)$. Moreover, if self-adjoint extensions of D exist, they may differ widely with respect to existence, uniqueness, regularity, and heat trace expansions. It is, therefore, our first task to characterize those self-adjoint extensions which behave nicely with respect to existence, uniqueness, and regularity.

3. Results for the model operator

Replacing in (2.1) $L^2(E_N)$ by an arbitrary Hilbert space, H, and $C^\infty(E_N)$ by the domain, H_1, of a self-adjoint operator A in H, we obtain the model operator

(3.1) $\qquad D = \gamma\left(\dfrac{d}{dx} + A\right)$ in $\mathcal{H}_0 := L^2(\mathbb{R}_+, H)$ with domain $C_0^\infty(\mathbb{R}_+, H_1)$.

We will have to deal with variable coefficients but for the purpose of this overview we will restrict ourselves to the constant coefficient case. Indeed, for most of the problems dealt with in this paper, operators with variable coefficients merely appear as perturbations of constant ones, in view of the Kato-Rellich Theorem.

On $C_0^\infty(\mathbb{R}_+, H_1)$ we clearly have

(3.2) $\qquad (Df, g)_{\mathcal{H}_0} - (f, Dg)_{\mathcal{H}_0} = \langle f(0), \gamma g(0) \rangle_H.$

Now if D is symmetric on a subspace, $\mathcal{D}^0$, of $C_0^\infty(\mathbb{R}_+, H_1)$ then it follows from (3.2) that, with $I - P$ the orthogonal projection onto $\overline{\mathcal{D}^0}$ in H, we have

(3.3a) $\qquad \mathcal{D}^0 \subset \mathcal{D}_P := \left\{ f \in C_0^\infty(\mathbb{R}_+, H_1) \mid Pf(0) = 0 \right\}$

and

(3.3b) $\qquad I - P \leq \gamma^* P \gamma.$

Moreover, $D_P := D \restriction \mathcal{D}_P$ is a symmetric extension of $D \restriction \mathcal{D}^0$. If we assume for a moment that H is of finite dimension then it is readily seen that D_P is essentially self-adjoint in $\mathcal{H}_0$ if and only if

(3.4) $\qquad I - P = \gamma^* P \gamma.$

Indeed, if $D_{\max}$ denotes $(D \upharpoonright C_0^\infty((0,\infty), H_1))^*$ then

$$(3.5) \qquad\qquad \mathcal{D}(D_{\max}) \subset H_{1,\mathrm{loc}}(\mathbb{R}_+, H),$$

and (3.2) remains valid with $D_{\max}$ in place of D, for $f, g \in \mathcal{D}(D_{\max})$.

An orthogonal projection, P, with (3.4) will be called γ–*symmetric*; it is easy to see that γ–symmetric projections – and hence self–adjoint extensions of D – exist if and only if

$$(3.6) \qquad\qquad \mathrm{sign}(i\gamma \upharpoonright \ker A) = 0.$$

As an illustration, note that $i\frac{d}{dx}$ does not admit self-adjoint extensions in $L^2(\mathbb{R}_+)$.

Returning to the general case, we meet the essential difficulty that (3.5) has no reasonable analogue. In particular, elements of $\mathcal{D}(D_{\max})$ do not admit H-valued restrictions to zero. To overcome this obstacle, we imitate the Sobolev scales $H_s(E_N)$ and $H_s(E)$ and their interplay in our abstract setting (which has some tradition in Analysis, cf. eg. [**15**, Chap. XIII]). $H_s(E_N)$ is replaced by

$$(3.7) \qquad \begin{aligned} H_s &:= H_s(\mathring{A}) \\ &:= \begin{cases} \mathcal{D}(|A|^s), \text{ equipped with the graph norms for } s \geq 0; \\ \text{a suitable dual of } H_{-s}(A), \text{ for } s < 0. \end{cases} \end{aligned}$$

We also need

$$H_\infty := H_\infty(A) := \bigcap_{s \in \mathbb{R}} H_s(A);$$

and

$$H_{-\infty} := H_{-\infty}(A) := \bigcup_{s \in \mathbb{R}} H_s(A).$$

Next we introduce, for $n \in \mathbb{Z}_+$,

$$(3.8a) \qquad \mathcal{H}_n := \mathcal{H}_n(\mathbb{R}_+, A) := \bigcap_{k=0}^{n} H_k(\mathbb{R}_+, H_{n-k}(A)),$$

where, for $i, j \in \mathbb{Z}_+$,

$$(3.8b) \qquad \begin{aligned} &H_i(\mathbb{R}_+, H_j(A)) \\ &:= \Big\{ f \in \mathcal{H}_0 \mid \Big(\frac{d}{dx}\Big)^l f \in L^2(\mathbb{R}_+, H_j(A)), \quad 0 \leq l \leq i \Big\}. \end{aligned}$$

By duality and interpolation, we then obtain a scale of Hilbert spaces, $\mathcal{H}_s = \mathcal{H}_s(\mathbb{R}_+, A), s \in \mathbb{R}$. Generalizing the classical Trace Theorem for Sobolev spaces, we have the following result about trace maps which will allow the formulation of boundary conditions.

THEOREM 3.1. *The map*

$$r : C_0^\infty(\mathbb{R}_+, H_\infty) \ni f \longmapsto f(0) \in H_\infty$$

extends by continuity to a map

$$r_s : \mathcal{H}_s \longrightarrow H_{s-1/2}, \quad s > 1/2,$$

and also to a map

$$r^* : \mathcal{D}(D_{\max}) \to H_{-1/2}.$$

Of course, the loss of regularity under the trace map requires the (continuous) extension of the boundary projections to the space $H_{-1/2}$. To deal with this, we introduce *operators of finite order* on the Hilbert scale $(H_s(A))_{s \in \mathbb{R}}$. Thus, a linear map, $B : H_\infty \to H_\infty$, is an operator of order $\mu \in \mathbb{R}$ if for each $s \in \mathbb{R}$ there is a constant $C(s)$ such that, for any $x \in H_\infty$,

$$(3.9) \qquad \|Bx\|_{H_s} \le C(s)\|x\|_{H_{s+\mu}}.$$

In particular, B extends to an element of $\mathcal{L}(H_s, H_{s-\mu})$ for all $s \in \mathbb{R}$. The totality of such operators forms the linear space $\mathrm{Op}^\mu(A)$. $\mathrm{Op}^{-\infty}(A) := \bigcap_{\mu \in \mathbb{R}} \mathrm{Op}^\mu(A)$ is called the space of *smoothing operators*.

Thus we will have to require that the boundary projections are elements of $\mathrm{Op}^0(A)$. It follows easily from (3.9) that $\mathrm{Op}^0(A)$ is a $*$-algebra but it is, in general, not *spectrally invariant* in the sense that $B \in \mathrm{Op}^0(A)$ and B invertible in $\mathcal{L}(H)$ implies $B^{-1} \in \mathrm{Op}^0(A)$. To allow for a minimum of functional constructions, we do need actually even more. We are forced to restrict attention to certain subalgebras, $\Psi^0(A) \subset \mathrm{Op}^0(A)$, satisfying the following two conditions.

(Ψ1) $\Psi^0(A)$ is a $*$-subalgebra of $\mathrm{Op}^0(A)$ with *holomorphic functional calculus*;

(Ψ2) $\Psi^0(A)$ contains an orthogonal projection, $P_+(A)$, satisfying

$$(3.10) \qquad I - P_+(A) = \gamma^* P_+(A)\gamma, \quad P_{(0,\infty)}(A) \le P_+(A) \le P_{[0,\infty)}(A).$$

Recall that an algebra, $\mathcal{A} \subset \mathcal{L}(H)$, has holomorphic functional calculus if for $B \in \mathcal{A}$ and f holomorphic in a neighbourhood of $\mathrm{spec}\, B$ (in $\mathcal{L}(H)$) we have $f(B) \in \mathcal{A}$, where $f(B)$ is defined by the Cauchy integral. Note also that the existence of $P_+(A)$ with (3.10) is equivalent to (3.6) in the finite dimensional case. In general, if $0 \notin \mathrm{spec}_{\mathrm{ess}} A$ then (3.6) is equivalent to the existence of a spectral projection of A satisfying (3.10).

Let us illustrate these conditions for the case where A is an elliptic differential operator on $C^\infty(E_N)$ and $N = \partial M$ as in Sec. 2. Then we have $H_s(A) \simeq H_s(E_N)$, and a natural choice of the algebra $\Psi^0(A)$ is the algebra of classical pseudodifferential operators on E_N, to be denoted by $\Psi^0_{\mathrm{cl}}(E_N)$. It follows from results of Seeley [18, Thm. 5] that $\Psi^0_{\mathrm{cl}}(E_N)$ has holomorphic functional calculus. Moreover, since $0 \notin \mathrm{spec}_{\mathrm{ess}} A$, we have to verify (3.6) to obtain a spectral projection, $P_+(A)$, of A fulfilling (3.10); but this is a consequence of the Cobordism Theorem. To see this, we split $H =: H_+ \oplus H_-$ according to the $\pm i$–eigenspaces of γ. In view of (2.2),

$$(3.11) \qquad A = \begin{pmatrix} 0 & A_- \\ A_+ & 0 \end{pmatrix},$$

and A_+ is a Fredholm operator with index

$$(3.12) \qquad \mathrm{ind}\, A_+ = \dim \ker A \cap \ker(\gamma - i) - \dim \ker A \cap \ker(\gamma + i).$$

Now it is straightforward to check that there exists an orthogonal projection $P_+(A) \in \mathrm{Op}^0(A)$ with the property (3.10) if and only if

$$(3.13) \qquad \mathrm{ind}\, A_+ = 0,$$

and this follows from the Cobordism Theorem (cf. the discussion after [9, Cor. 3.6]).

Again from Seeley's work, we deduce that $P_+(A) \in \Psi^0_{\mathrm{cl}}(E_N)$ so (Ψ1), (Ψ2) are satisfied in a natural way.

Now we are in the position to formulate our results for the model operator. The main theorem concerning regularity reads as follows.

THEOREM 3.2. *Let H be a Hilbert space and A a self-adjoint operator in H. Assume, moreover, that an algebra, $\Psi^0(A) \subset \mathrm{Op}^0(A)$, is given with the properties ($\Psi 1$) and ($\Psi 2$).*

Then D_P with domain (3.3a) is essentially self-adjoint in $L^2(\mathbb{R}_+, H)$ for any orthogonal projection $P \in \Psi^0(A)$ with the properties

$$(3.4) \qquad\qquad \gamma^* P \gamma = I - P$$

and

$$(3.14) \qquad\qquad (P, P_+(A)) \text{ is a Fredholm pair.}$$

The domain of the closure of D_P is $\mathcal{D}(D_P) = \{ f \in \mathcal{H}_1(\mathbb{R}_+, A) \mid Pf(0) = 0 \}$.

Conversely, if A is discrete then the self-adjointness of D_P on $\{ f \in \mathcal{H}_1(\mathbb{R}_+, A) \mid Pf(0) = 0 \}$ implies (3.4) and (3.14).

We note that the orthogonal projection $P_-(A) = I - P_+(A) \in \Psi^0(A)$ obviously does not satisfy (3.14). However, it can be shown that $D_{P_-(A)}$ is essentially self–adjoint with domain $\mathcal{D}(D_{P_-(A)}) \supsetneq \{ f \in \mathcal{H}_1(\mathbb{R}_+, A) \mid Pf(0) = 0 \}$. Hence the "self–adjointness" in the last statement of the Theorem cannot be replaced by "essentially self-adjoint on $\mathcal{D}_P$".

Recall that a pair of (orthogonal) projections, (P_1, P_2), in H is said to form a *Fredholm pair* if the map

$$P_2 : P_1(H) \longrightarrow P_2(H)$$

is Fredholm. This is easily seen to be equivalent to the fact that

$$(3.15a) \qquad P_2 P_1(H) \text{ (and hence } P_1 P_2(H)) \text{ is closed in } H$$

and

$$(3.15b) \qquad \dim(\ker P_2 \cap \mathrm{im}\, P_1) + \dim(\ker P_1 \cap \mathrm{im}\, P_2) < \infty$$

(such that (P_1, P_2) is Fredholm if and only if so is (P_2, P_1)). In this case, one calls

$$(3.16) \qquad \mathrm{ind}(P_1, P_2) := \dim(\ker P_2 \cap \mathrm{im}\, P_1) - \dim(\ker P_1 \cap \mathrm{im}\, P_2)$$

the *index of the pair* (P_1, P_2); cf. [**14**, IV.4.1], [**6**], [**7**, Sec. 24], [**5**].

The proof of Theorem 3.2 is technically complicated and cannot be described here in detail. We have to interpolate various abstract concepts of regularity such that we can show their mutual equivalence step by step.

We can view Theorem 3.2 as the analogue of (1.1) for the model operator. Taking advantage of the self-adjointness of D_P we can try to satisfy (1.2) by setting

$$(3.17) \qquad\qquad Q := \int_{|\lambda| \geq 1} \lambda^{-1} dE(\lambda),$$

where $E(\lambda) = E_{D_P}(\lambda), \lambda \in \mathbb{R}$, denotes the spectral resolution of D_P. From our abstract regularity with respect to the Sobolev scale $\mathcal{H}_s(\mathbb{R}_+, A)$, $s \in \mathbb{R}$, and a standard compactness argument we then derive the following analogue of (1.2) and (1.3).

THEOREM 3.3. *We assume the situation of Theorem 3.2 and, in addition, that A is discrete. For $\phi \in C_0^\infty(\mathbb{R})$ with $\phi = 1$ near 0 we put $Q_\phi := \phi Q$. Then Q_ϕ maps into $\mathcal{D}(D_P)$ and there are compact operators, $K_{r/l,\phi}$, in $\mathcal{H}$ such that*

$$(3.18) \qquad D_P Q_\phi = \phi - K_{r,\phi}, \qquad Q_\phi D_P = \phi - K_{l,\phi}.$$

Moreover, Q_ϕ is of order -1 and $K_{r/l,\phi}$ of order $-\infty$ with respect to the Sobolev scale $\mathcal{H}_s(\mathbb{R}_+, A), s \in \mathbb{R}$.

We have pointed out that, for the purposes of regularity theory, we may treat variable coefficients as a perturbation of the constant coefficient case; the same is true for index theory, by deformation. As in [9], a basic tool of our analysis is the analogue of a formula due to Sommerfeld, expressing the heat kernel of the model operator $D_{P_+(A)} =: D_{P_+}$ for $x, y, t > 0$,

$$(3.19) \qquad \begin{aligned} e^{-tD_{P_+}^2}&(x,y) \\ &= (4\pi t)^{-1/2} \left(e^{-(x-y)^2/4t} + (I - 2P_+)e^{-(x+y)^2/4t} \right) e^{-tA^2} \\ &\quad + (\pi t)^{-1/2}(I - P_+) \int_0^\infty e^{-(x+y+z)^2/4t} A e^{Az - tA^2} dz. \end{aligned}$$

In order to derive a reasonable index formula, we assume now that $(A + i)^{-1} \in \mathcal{L}_p(H)$ (the Schatten–von Neumann class) for some $p > 0$, and that

$$(3.20) \qquad \eta(A; s) := \frac{1}{\Gamma\left(\frac{s+1}{2}\right)} \int_0^\infty t^{(s-1)/2} \operatorname{tr}_H\left[A e^{-tA^2}\right] dt$$

extends to a meromorphic function in $\mathbb{C}$ without a pole at 0. Then it is not difficult to derive from (3.19) the following result which computes the "boundary contribution" to the index. Recall that $\omega := \widetilde{\omega} \restriction E$ is the involution defining the index. Then ω has to commute with A and P, and we put

$$(3.21) \qquad A^+ := A\frac{1}{2}(\omega + I), \quad P^+ := P\frac{1}{2}(\omega + I).$$

Furthermore, $\underset{t \to 0+}{\operatorname{LIM}} f(t)$ denotes the constant term in the asymptotic expansion of f, and $\eta(A^+) := \eta(A^+; 0)$.

THEOREM 3.4. *Under the assumptions of Theorem 3.3, let P also commute with ω and A,*

$$(3.22) \qquad [P, A] = [P, \omega] = 0.$$

Then we have, for any $\phi \in C_0^\infty(\mathbb{R})$ with $\phi = 1$ in a neighborhood of 0,

$$(3.23) \qquad \begin{aligned} \underset{t \to 0+}{\operatorname{LIM}} \operatorname{tr}\left[\phi \omega e^{-tD_P^2}\right] &= -\frac{1}{2}\left(\eta(A^+) + \dim \ker A^+\right) + \operatorname{ind}(P_{\geq 0}(A^+), P^+) \\ &=: \xi(A^+) + \operatorname{ind}(P_{\geq 0}(A^+), P^+). \end{aligned}$$

It turns out that regular boundary projections other than $P_+(A)$ are quite useful. Moreover, their functional analytic characterization shows that they form a convenient tool for "glueing indices". We have used this already in [9] for the more complicated case of η–invariants; we recall briefly what is involved.

Consider the model operator (3.1) on $L^2(\mathbb{R}, H)$ where it is essentially self–adjoint. The reflection isometry (generated by $\sigma(x) = -x$),

$$\Phi_\sigma : L^2(\mathbb{R}, H) \longrightarrow L^2(\mathbb{R}_+, H \oplus H), \quad f \longmapsto (f \restriction \mathbb{R}_+, f \circ \sigma \restriction \mathbb{R}_+),$$

transforms this operator unitarily to a model operator on $\mathbb{R}_+$,

$$(3.24a) \qquad\qquad D = \widetilde{\gamma}\left(\frac{d}{dx} + \widetilde{A}\right),$$

with domain $C_0^\infty(\mathbb{R}_+, H_1 \oplus H_1)$ in $L^2(\mathbb{R}_+, H \oplus H)$, where

$$(3.24b) \qquad\qquad \widetilde{\gamma} = \begin{pmatrix} \gamma & 0 \\ 0 & -\gamma \end{pmatrix} \quad \text{and} \quad \widetilde{A} = \begin{pmatrix} A & 0 \\ 0 & -A \end{pmatrix}.$$

The boundary condition (the smooth transmission condition) simply becomes, for $u = (u_1, u_2) \in C_0^\infty(\mathbb{R}_+, H_1 \oplus H_1)$,

$$(3.24c) \qquad\qquad u_1(0) = u_2(0).$$

The subspace of $H \oplus H$ defined by (3.24c) can be viewed as the $+1$–eigenspace of the involution

$$(3.25) \qquad\qquad \tau := \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix},$$

and if P is any orthogonal projection in $H \oplus H$ satisfying

$$(3.26) \qquad\qquad \tau P = (I - P)\tau,$$

then

$$(3.27a) \qquad\qquad \alpha := P - (I - P)$$

is a second self–adjoint involution with

$$(3.27b) \qquad\qquad \tau\alpha = -\alpha\tau.$$

Now we define a family of unitaries by

$$(3.28a) \qquad\qquad U(\theta) := \cos\theta I + \sin\theta\alpha\tau, \quad |\theta| < \pi/2,$$

and a corresponding family of projections by

$$(3.28b) \qquad\qquad \begin{aligned} P(\theta) &:= U(\theta)^* P U(\theta) \\ &= \cos^2\theta P + \sin^2\theta(I - P) + \sin\theta\cos\theta\tau. \end{aligned}$$

Clearly, $P(\pi/4)$ projects onto the $+1$–eigenspace of τ, so the family (3.28b) is a deformation of (3.24c). In particular, from $\tau\widetilde{A} + \widetilde{A}\tau = 0$ we see that

$$(3.29) \qquad\qquad P = P_+(\widetilde{A}) := \begin{pmatrix} P_+(A) & 0 \\ 0 & I - P_+(A) \end{pmatrix}$$

is an admissible choice, and we obtain a continuous deformation from the Atiyah–Patodi–Singer boundary condition - which decouples D - to the smooth transmission boundary condition. Therefore, the following result is of interest for index calculations.

THEOREM 3.5. *If P is regular, so is $P(\theta)$ for $|\theta| < \pi/2$, and the family $D_{P(\theta)}$ is graph continuous in $(-\pi/2, \pi/2)$.*

Index theorems for the model operator on finite or infinite intervals in $\mathbb{R}$ have also been used frequently in recent years, cf. eg. [16]. The methods described so far are the starting point for a systematic abstract study of this topic. Thus, let us consider the operator

$$(3.30) \qquad\qquad D_{P,Q}^{a,b} := \frac{d}{dx} + A(x)$$

with domain (cf. (3.8a)) $\mathcal{D}_{P,Q}^{a,b} := \{ f \in \mathcal{H}_1([a,b], A) \mid Pf(a) = (I-Q)f(b) = 0 \}$ in $L^2([a,b], H)$. Now it is of importance that we admit variable coefficients. Precisely, we assume that $A \in C^\infty([a,b], \mathcal{L}(H_1, H))$ and that each $A(x)$ is self-adjoint in H with domain H_1, and a Fredholm operator. It is well known that the index of $D_{P,Q}^{a,b}$ is related to the spectral flow of the family $A(x)$ across $[a,b]$, to be denoted by $\mathrm{sf}_{[a,b]} A$ (cf. part II of [4] for the definition and the main properties of sf A). Our main result here has various obvious corollaries like a formula for the spectral flow and for the variation of ξ-invariants; it reads as follows.

THEOREM 3.6. *Let A be as above and assume that P, Q are orthogonal projections in H such that $(P_{\geq 0}(A(a)), P)$ and $(P_{\geq 0}(A(b)), Q)$ are Fredholm pairs. Then (the closure of) $D_{P,Q}^{a,b}$ is a Fredholm operator with*

$$
\begin{aligned}
\text{(3.31)} \quad \mathrm{ind}\, D_{P,Q}^{a,b} = &-\frac{1}{\sqrt{\pi}} \int_a^b \underset{t\to 0+}{\mathrm{LIM}}\, t^{1/2}\, \mathrm{tr}_H\big[A'(x)e^{-tA(x)^2}\big]\,dx \\
&- \xi(A(a)) + \mathrm{ind}(P_{\geq 0}(A(a)), P) \\
&+ \xi(A(b)) - \mathrm{ind}(P_{\geq 0}(A(b)), Q) \\
= &\ \mathrm{sf}_{[a,b]} A + \mathrm{ind}(P_{\geq 0}(A(a)), P) - \mathrm{ind}(P_{\geq 0}(A(b)), Q).
\end{aligned}
$$

Finally, we turn to the asymptotic expansion of the heat trace. Again, we obtain by simple abstract methods a substantial result, without using any pseudodifferential technology but, for the time being, our result is far from being best possible. Thus, we now restrict attention to projections, P, which satisfy the assumptions in Theorem 3.2 and, in addition,

$$
\text{(3.32)} \qquad\qquad P - P_+(A) \in \mathrm{Op}^{-1}(A).
$$

Now, for the expansion problem variable coefficients are considerably more difficult than constant ones. We thus allow a family, $(A(x))_{x \geq 0}$, satisfying the conditions needed in Theorem 3.6 and also, with $A := A(0)$,

$$
\text{(3.33)} \qquad\qquad A(x) \equiv A \quad \text{for } x \geq x_0 > 0.
$$

Since we need the expansion result only near the boundary $x = 0$ in most applications, (3.33) does not mean an essential restriction, but (3.32) does.

To obtain complete asymptotic expansions, we need of course to assume expansion properties for the family $(A(x))$. These assumptions are somewhat technical so we refrain from stating them here in detail, it may suffice to assert that they are satisfied in the most prominent case when $\Psi^0(A) = \Psi_{\mathrm{cl}}^0(E_N)$, for some compact Riemannian manifold N and some hermitian bundle $E_N \to N$. Then we obtain

THEOREM 3.7. *Under the assumptions mentioned above, we obtain for any $\phi \in C_0^\infty(\mathbb{R}_+)$ an asymptotic expansion*

$$
\text{(3.34)} \qquad \mathrm{tr}_{L^2(\mathbb{R}_+, H)}\big[\phi e^{-tD_P^2}\big] \sim_{t\to 0+} \sum_{\substack{j \geq 0 \\ 0 \leq k \leq 1}} a_{jk}(P, \phi) t^{j/2-p} \log^k t,
$$

for some $p > 0$ depending on A. If $j/2 - p \leq 0$ we have $a_{j1} = 0$.

4. Results for manifolds with boundary

It is not difficult to translate Theorems 3.2 through 3.6 into statements on D and the Sobolev scales $H_s(E)$ and $H_s(E_N), s \in \mathbb{R}$. First, we only need to make Lemma 2.1 somewhat more explicit. For this, we introduce, on U, the global coordinate

$$(4.1) \qquad x(p) := \mathrm{dist}(p, N), \quad p \in N,$$

and denote by

$$(4.2) \qquad \Phi : L^2(E \restriction U) \longrightarrow L^2((-\varepsilon_0, \varepsilon_0), L^2(E_N))$$

the isometry implicit in Lemma 2.1. Then we have the properties

$$(4.3\mathrm{a}) \qquad \psi \Phi u = \Phi\big((\psi \circ x)u\big), \qquad \psi \in C^\infty(-\varepsilon_0, \varepsilon_0), u \in L^2(E \restriction U),$$

$$(4.3\mathrm{b}) \qquad (\Phi u)(0) = u \restriction N, \qquad u \in C^\infty(E \restriction \overline{M}),$$

$$(4.3\mathrm{c}) \qquad \Phi\big((\psi \circ x)H_s(E)\big) = \psi \mathcal{H}_s, \qquad \psi \in C_0^\infty(-\varepsilon_0, \varepsilon_0), s \in \mathbb{R},$$

which allow us to localize near N and to transfer regularity.

To formulate the boundary conditions, we restrict attention to orthogonal projections in $L^2(E_N)$ which are classical pseudodifferential operators i.e. from now on we choose $\Psi^0(A) = \Psi_{\mathrm{cl}}^0(E_N)$, as indicated above. In the theory of boundary value problems for linear elliptic differential operators, it was observed by Calderón [10] that a prominent role is played by an idempotent, $C^+ \in \Psi_{\mathrm{cl}}^0(E_N)$, with the property that

$$(4.4) \qquad \begin{aligned} C^+(H_s(E_N)) &= N_s(E_N) \\ &:= \big\{ u \in H_s(E_N) \mid u = \widetilde{u} \restriction N \text{ for } \widetilde{u} \in H_{s+1/2}(E) \text{ with } D\widetilde{u} = 0 \big\} \end{aligned}$$

for all $s \in \mathbb{R}; C^+$ is called the *Calderón projector* (cf. [17, 19], a comprehensive summary can be found in [13, Appendix]). One checks that

$$(4.5) \qquad C^+ - P_+(A) \in \Psi_{\mathrm{cl}}^{-1}(E_N)$$

which explains the importance of the Atiyah–Patodi–Singer boundary condition. In order to obtain boundary conditions which define Fredholm operators (as in (1.2), (1.3)), Seeley introduced the notion of "well-posed" boundary condition [19]. Combining the results described so far with a microlocal argument, we obtain the following optimal version of Seeley's result, as a consequence of our general theory.

THEOREM 4.1. *Let $P \in \Psi_{\mathrm{cl}}^0(E_N)$ be an orthogonal projection in $L^2(E_N)$ satisfying* (3.4).

Then D with domain $\mathcal{D}_P := \big\{ f \in H_1(\widetilde{E} \restriction \overline{M}) \mid P(f \restriction N) = 0 \big\}$ is self-adjoint in $L^2(E)$ if and only if P is well-posed in the sense of Seeley. This, in turn, is equivalent to the fact that $(P, P_+(A))$ is a Fredholm pair.

In this case, denote by D_P the closure of $D \restriction \mathcal{D}_P$. Then there are a bounded operator, Q, and compact operators, K_r, K_l, in $L^2(E)$ such that Q maps into $\mathcal{D}(D_P)$ and

$$D_P Q = I - K_r, \quad Q D_P = I - K_l.$$

Moreover, with respect to the Sobolev scale $H_s(E), s \in \mathbb{R}, Q$ is of order -1 and $K_{r/l}$ of order $-\infty$.

For index theorems in the framework of Theorem 3.7, we can reduce the computations to the situation addressed in Theorem 3.4, in view of the deformation properties of Fredholm pairs in $\Psi^0_{\mathrm{cl}}(E_N)$ (here (Ψ1) is important) and the Local Index Theorem. Recall that the latter asserts that

$$\lim_{t \to 0+} \mathrm{tr}_{\widetilde{E}} \big[\widetilde{\omega} e^{-t\widetilde{D}^2}(p,p) \big] \, \mathrm{vol}_M(p) =: \alpha_D(p)$$

exists for any $p \in \widetilde{M}$ and coincides with the Atiyah–Singer integrand. We obtain the following result which contains the Atiyah–Patodi–Singer Theorem as well as a result of Agranovich and Dynin [**1**].

THEOREM 4.2. *Under the assumptions of Theorem 3.7 we obtain*

$$(4.6) \qquad \mathrm{ind}\, D_{P,+} = \int_M \alpha_D + \int_N \beta_D - \xi(A(0)^+) + \mathrm{ind}(P_{\geq 0}(A(0)^+), P^+).$$

Here, $(A(x))_{x \geq 0}$ is the family obtained from $\widetilde{D}$ by separation of variables as in Lemma 2.1, and β_D is given by a universal expression in the derivatives $A^{(j)}(0)$.

Geometric formulas for β_D (for specific $\widetilde{D}$) have been given by Gilkey [**12**, Chap. 3,10]; they involve the second fundamental form of N.

Theorem 3.5 has also a very useful application in the present context to a "glueing formula" for indices. This is meant to say that we emphasize the constancy of the index along the curve given by $D_{P(\theta),+}$, for $0 \leq \theta \leq \pi/4$, decoupling the problem at $\theta = 0$.

More precisely, in the situation described at the beginning of Sec. 2, M is decomposed as the union of two manifolds with boundary which we denote by M^+ and M^-,

$$(4.7) \qquad\qquad\qquad M = M^+ \cup M^- \cup N.$$

Here, the orientation of N is as boundary of M^+, hence the opposite of the boundary orientation induced by M^-. The isomophism (4.2) in Lemma 2.1 is normalized in such a way that

$$(4.8) \qquad\qquad \Phi(L^2(\widetilde{E} \upharpoonright U \cap M^+)) = L^2((0, \varepsilon_0), L^2(E_N)).$$

Then we have the following result relating the index of $\widetilde{D}$ to the index of boundary value problems on M^+ and M^- (which we add in the notation of the operators, for clarity).

THEOREM 4.3. *Let $P \in \Psi^0_{\mathrm{cl}}(E_N)$ satisfy (3.4) and (3.14), and assume that P commutes with ω. Then*

$$(4.9) \qquad\qquad\qquad \mathrm{ind}\, \widetilde{D}_+ = \mathrm{ind}\, D^{M^+}_{P,+} + \mathrm{ind}\, D^{M^-}_{I-P,+}.$$

Let us elaborate a little bit on the formula (4.9). To $D^{M^+}_{P,+}$ we can directly apply the index formula (4.6) which makes (implicitly) use of the chosen orientation through Lemma 2.1, whereas for $D^{M^-}_{I-P,+}$ we have to change the orientation of N. In (4.6), this amounts to changing the sign of β_D and replacing $A(0)^+$ by $-A(0)^+$. Now an easy computation gives

$$\mathrm{ind}(P_{\geq 0}(-A(0)^+), I - P^+) = \mathrm{ind}(I - P_{>0}(A(0)^+), I - P^+)$$
$$= -\,\mathrm{ind}(P_{>0}(A(0)^+), P^+)$$

and

$$\begin{aligned}
\operatorname{ind}(P_{\geq 0}(A(0)^+), P^+) &= \operatorname{ind}(P_{\geq 0}(A(0)^+), P_{>0}(A(0)^+)) \\
&\quad + \operatorname{ind}(P_{>0}(A(0)^+), P^+) \\
&= \dim \ker A(0)^+ + \operatorname{ind}(P_{>0}(A(0)^+), P^+).
\end{aligned}$$

Since $\eta(-A) = -\eta(A)$, we see that (4.9) and (4.6) combine to

$$\operatorname{ind} \widetilde{D}_+ = \int_M \alpha_D,$$

as it must be.

We remark that (4.9) remains true also in more general situations where $\widetilde{M}$ need not be compact (but, of course, $\widetilde{D}$ has to be Fredholm).

Theorem 3.7 and 4.3 can be used to give very simple and transparent proofs of various known results, notably the Cobordism Theorem and index theorems of Callias type. As mentioned before, the model operator does not "see" compactness; as an example of its wider applicability, we mention a very simple proof of the covering space version of the Atiyah–Patodi–Singer Theorem, due to Ramachandran.

Finally, we turn to the asymptotic expansion of the heat trace, based on Theorem 3.7. Applied to the situation at hand, our result is not as strong as the recent expansion theorem proved by G. Grubb [13] even though we employ a much more elementary technique. Nevertheless, let us state Grubb's result for completeness (our proof needs (3.32) for the time being).

THEOREM 4.4. *Let $P \in \Psi^0_{\mathrm{cl}}(E_N)$ be well-posed and satisfy (3.4). Then there is an asymptotic expansion*

$$(4.10) \qquad \operatorname{tr}\left[\omega^i D_P^j e^{-t D_P^2}\right] \sim_{t \to 0+} \sum_{\substack{k \geq 0 \\ l=0,1}} a_{kl}^{ij}(D, P) t^{(k-m-j)/2} \log^l t.$$

Here,

$$(4.11) \qquad\qquad a_{k1}^{ij} = 0 \quad \text{if } k - m - j < 0.$$

Under the more restrictive assumption (3.32) we can show that (4.11) holds even for $k - m - j \leq 0$; this is relevant for the study of the (ζ-regularized) determinant of D_P^2 and D_P.

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HUMBOLDT UNIVERSITÄT ZU BERLIN, INSTITUT FÜR MATHEMATIK, UNTER DEN LINDEN 6, D–10099 BERLIN
E-mail address: bruening@mathematik.hu-berlin.de

HUMBOLDT UNIVERSITÄT ZU BERLIN, INSTITUT FÜR MATHEMATIK, UNTER DEN LINDEN 6, D–10099 BERLIN
Current address: Universität Bonn, Mathematisches Institut, Beringstr. 1, D–53115 Bonn
E-mail address: lesch@mathematik.hu-berlin.de, lesch@math.uni-bonn.de