THE Ξ OPERATOR AND ITS RELATION TO KREIN'S SPECTRAL SHIFT FUNCTION

FRITZ GESZTESY AND KONSTANTIN A. MAKAROV

Abstract. We explore connections between Krein's spectral shift function $\xi(\lambda, H_0, H)$ associated with the pair of self-adjoint operators (H_0, H), $H = H_0 + V$ in a Hilbert space $\mathcal{H}$ and the recently introduced concept of a spectral shift operator $\Xi(J + K^*(H_0 - \lambda - i0)^{-1}K)$ associated with the operator-valued Herglotz function $J + K^*(H_0 - z)^{-1}K$, $\mathrm{Im}(z) > 0$ in $\mathcal{H}$, where $V = KJK^*$ and $J = \mathrm{sgn}(V)$. Our principal results include a new representation for $\xi(\lambda, H_0, H)$ in terms of an averaged index for the Fredholm pair of self-adjoint spectral projections $(E_{J+A(\lambda)+tB(\lambda)}((-\infty, 0)), E_J((-\infty, 0)))$, $t \in \mathbb{R}$, where $A(\lambda) = \mathrm{Re}(K^*(H_0 - \lambda - i0)^{-1}K)$, $B(\lambda) = \mathrm{Im}(K^*(H_0 - \lambda - i0)^{-1}K)$ a.e. Moreover, introducing the new concept of a trindex for a pair of operators (A, P) in $\mathcal{H}$, where A is bounded and P is an orthogonal projection, we prove that $\xi(\lambda, H_0, H)$ coincides with the trindex associated with the pair $(\Xi(J + K^*(H_0 - \lambda - i0)^{-1}K), \Xi(J))$. In addition, we discuss a variant of the Birman-Krein formula relating the trindex of a pair of Ξ-operators and the Fredholm determinant of the abstract scattering matrix.

We also provide a generalization of the classical Birman-Schwinger principle, replacing the traditional eigenvalue counting functions by appropriate spectral shift functions.

1. Introduction

In order to facilitate a description of the content of this paper we briefly introduce the notation used throughout this manuscript. The open complex upper half-plane is abbreviated by $\mathbb{C}_+ = \{z \in \mathbb{C} \,|\, \mathrm{Im}(z) > 0\}$; the symbols $\mathcal{H}, \mathcal{K}$ represent complex separable Hilbert spaces and $I_{\mathcal{H}}$ the corresponding identity operator in $\mathcal{H}$. Moreover, we denote by $\mathcal{B}(\mathcal{H})$, $\mathcal{B}_\infty(\mathcal{H})$, the Banach spaces of bounded and compact operators in $\mathcal{H}$ and by $\mathcal{B}_p(\mathcal{H})$, $p \geq 1$ the standard Schatten-von Neumann trace ideals (cf., [22], [47]). Real and imaginary parts of an operator T with $\mathrm{dom}(T) = \mathrm{dom}(T^*)$ are defined as usual by $\mathrm{Re}(T) = (T + T^*)/2$ and $\mathrm{Im}(T) = (T - T^*)/(2i)$; the spectrum, essential and absolutely continuous spectrum of T is abbreviated by $\mathrm{spec}(T)$, $\mathrm{ess.spec}(T)$, and $\mathrm{ac.spec}(T)$, respectively. For a self-adjoint operator $H = H^*$ in $\mathcal{H}$, the associated family of strongly right-continuous orthogonal spectral projections of H in $\mathcal{H}$ is denoted by $\{E_H(\lambda)\}_{\lambda \in \mathbb{R}}$.

Before describing the content of each section, we briefly summarize the principal results of this paper. Let H_0 and $H = H_0 + V$ be self-adjoint operators in $\mathcal{H}$ with $V = V^* \in \mathcal{B}_1(\mathcal{H})$ and denote by $\xi(\lambda, H_0, H)$ Krein's spectral shift function associated with the pair (H_0, H), uniquely defined for a.e. $\lambda \in \mathbb{R}$ by $\xi(\cdot, H_0, H) \in L^1(\mathbb{R}; d\lambda)$ and

$$\mathrm{tr}((H - z)^{-1} - (H_0 - z)^{-1}) = -\int_{\mathbb{R}} d\lambda\, \xi(\lambda, H_0, H)(\lambda - z)^{-2}, \quad z \in \mathbb{C} \backslash \mathbb{R}. \tag{1.1}$$

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Denoting by $\mathrm{index}(P,Q)$ the index of a Fredholm pair of orthogonal projections in $\mathcal{H}$, one of our principal results represents $\xi(\lambda,H_0,H)$ as an averaged index for the Fredholm pair of projections $(E_{J+A(\lambda)+tB(\lambda)}((-\infty,0)),E_J((-\infty,0)))$, $t\in\mathbb{R}$, as follows (cf. Theorem 5.5),

$$\xi(\lambda,H_0,H)=\frac{1}{\pi}\int_{\mathbb{R}}dt\frac{\mathrm{index}\big(E_{J+A(\lambda)+tB(\lambda)}((-\infty,0)),E_J((-\infty,0))\big)}{1+t^2} \tag{1.2}$$

for a.e. $\lambda\in\mathbb{R}$. Here $V=H-H_0$ is decomposed as

$$V=KJK^*,\quad K\in\mathcal{B}_2(\mathcal{H}),\ J=\mathrm{sgn}(V) \tag{1.3}$$

and

$$A(\lambda)=\operatorname*{n-lim}_{\varepsilon\downarrow 0}\mathrm{Re}(K^*(H_0-\lambda-i\varepsilon)^{-1}K), \tag{1.4}$$

$$B(\lambda)=\operatorname*{n-lim}_{\varepsilon\downarrow 0}\mathrm{Im}(K^*(H_0-\lambda-i\varepsilon)^{-1}K)\text{ for a.e. }\lambda\in\mathbb{R}. \tag{1.5}$$

In the special sign-definite case where $J=\pm I_{\mathcal{H}}$, formula (1.2) implies a result of Pushnitskii [40] (cf. Corollary 5.6).

Next, observing that the trace class-valued operator $K^*(H_0-z)^{-1}K$, $z\in\mathbb{C}_+$ has nontangential boundary values $K^*(H_0-\lambda-i0)^{-1}K$ for a.e. $\lambda\in\mathbb{R}$ in $\mathcal{B}_p(\mathcal{H})$-topology for each $p>1$, but in general not in the trace norm $\mathcal{B}_1(\mathcal{H})$-topology, we introduce the notion of a trindex, $\mathrm{trindex}(\cdot,\cdot)$, for a pair of operators (A,Q) in $\mathcal{H}$, where $A\in\mathcal{B}(\mathcal{H})$ is bounded and $Q=Q^*=Q^2$ is an orthogonal projection in $\mathcal{H}$, as follows: the pair (A,Q) is said to have a *trindex*, denoted by $\mathrm{trindex}(A,Q)$, if there exists an orthogonal projection P in $\mathcal{H}$ such that $(A-P)\in\mathcal{B}_1(\mathcal{H})$ and (P,Q) is a Fredholm pair of orthogonal projections in $\mathcal{H}$. In this case one then defines,

$$\mathrm{trindex}(A,Q)=\mathrm{tr}(A-P)+\mathrm{index}(P,Q). \tag{1.6}$$

Introducing the spectral shift operator $\Xi(T)=(1/\pi)\mathrm{Im}(\log(T))$ for a bounded dissipative operator T, with T^{-1} also bounded in $\mathcal{H}$, our second principal result (cf. Theorem 5.3) identifies $\xi(\lambda,H_0,H)$ with the trindex of the pair $(\Xi(J+K^*(H_0-\lambda-i0)^{-1}K),\Xi(J))$, that is,

$$\xi(\lambda,H_0,H)=\mathrm{trindex}(\Xi(J+K^*(H_0-\lambda-i0)^{-1}K),\Xi(J))\text{ for a.e. }\lambda\in\mathbb{R}. \tag{1.7}$$

The trindex representation (1.7) paves the way for introducing a generalized spectral shift function to be discussed in detail in Section 5. We also show that the averaging formula (1.2) should be viewed as a generalized Birman-Schwinger principle

$$\xi(\lambda,H_0,H)=\frac{1}{\pi}\int_{\mathbb{R}}dt\,\frac{\widehat{\xi}(0_-,J+A(\lambda)+tB(\lambda),J)}{1+t^2}\text{ for a.e. }\lambda\in\mathbb{R}, \tag{1.8}$$

where $\widehat{\xi}(\cdot,J+A(\lambda)+tB(\lambda),J)$ denotes the generalized spectral shift function associated with the pair $(J+A(\lambda)+tB(\lambda),J)$, $t\in\mathbb{R}$.

Next we turn to a description of the content of each section. In Section 2 we briefly review basic properties of the index of a Fredholm pair of projections in $\mathcal{H}$ (mainly following [3], see also [1], [24], [25]) and then present a discussion of the notion of trindex and some of its properties. Section 3 is devoted to the concept of a Ξ-operator as recently introduced in [19] and further discussed in [18]. More precisely, if T is a bounded dissipative operator with $T^{-1}\in\mathcal{B}(\mathcal{H})$, then $\Xi(T)$ is defined by

$$\Xi(T)=\frac{1}{\pi}\mathrm{Im}(\log(T)). \tag{1.9}$$

Section 3 also studies sufficient conditions on $A = A^* \in \mathcal{B}_\infty(\mathcal{H})$ and $0 \le B \in \mathcal{B}_1(\mathcal{H})$ to guarantee $(\Xi(S+A+iB) - \Xi(S+A)) \in \mathcal{B}_1(\mathcal{H})$ for given $S = S^* \in \mathcal{B}(\mathcal{H})$. Section 4, the technical core of this paper, provides a discussion of averaged Fredholm indices. Introducing the family of normal trace class operators,

$$\mathcal{A}(z) = B^{1/2}(S + zB)^{-1}B^{1/2}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{1.10}$$

where $S = S^* \in \mathcal{B}(\mathcal{H})$, $S^{-1} \in \mathcal{B}(\mathcal{H})$, $0 \le B \in \mathcal{B}_1(\mathcal{H})$, associated with the (dissipative) family of operator-valued Herglotz functions

$$T(z) = S + zB, \quad z \in \mathbb{C}_+ \tag{1.11}$$

(i.e., T is analytic in $\mathbb{C}_+$ and $\operatorname{Im}(T(z)) \ge 0$ for $z \in \mathbb{C}_+$), we prove

$$\operatorname{tr}(\log(T(z)) - \log(S)) = \sum_{k=1}^{\infty} m_k \int_0^1 d\tau\, \frac{z\lambda_k}{1 + \tau z \lambda_k}, \tag{1.12}$$

(cf. Theorem 4.3), where $\{\lambda_k\}_{k\in\mathbb{N}} \subset \mathbb{R}$ is the set of eigenvalues with associated multiplicities $\{m_k\}_{k\in\mathbb{N}}$ of the self-adjoint trace class operator $B^{1/2}S^{-1}B^{1/2}$. This then yields our principal result (Theorem 4.10) relating the trindex of the pair $(\Xi(S + A + iB), \Xi(S))$ and the averaged Fredholm index $n(t) = \operatorname{index}(\Xi(S + A + tB), \Xi(S))$, $t \in \mathbb{R}$, as

$$\operatorname{trindex}(\Xi(S + A + iB), \Xi(S)) = \frac{1}{\pi}\int_{\mathbb{R}} \frac{dt\, n(t)}{1 + t^2}. \tag{1.13}$$

Moreover, we provide a version of the Birman-Krein formula relating the left-hand side of (1.13) and the determinant of the abstract scattering matrix

$$\exp(-2\pi i \operatorname{trindex}(\Xi(S + A + iB), \Xi(S))) = \det(I_{\mathcal{H}} - 2iB^{1/2}(S + A + iB)^{-1}B^{1/2}). \tag{1.14}$$

Section 5 finally presents the applications of our formalism to Krein's spectral shift function $\xi(\lambda, H_0, H)$ as discussed in (1.2), (1.7), and (1.8).

In conclusion, we note that Krein's spectral shift function [30]–[34], a concept originally introduced by Lifshits [35], [36], continues to generate considerable interest. Without repeating the extensive bibliography recently provided in [19], we remark that the spectral shift function plays a fundamental role in scattering theory, (relative) index theory, spectral averaging and its application to localization properties of random Hamiltonians, eigenvalue counting functions and spectral asymptotics, semi-classical approximations, and trace formulas for one-dimensional Schrödinger and Jacobi operators. A very selective list of recent pertinent references includes, for instance, [8], [14], [16]–[18], [20], [29], [37], [40]–[42], [44], [45], [48], [49]. For many more references the interested reader can consult the 1993 reviews by Birman and Yafaev [11], [12], and [18], [19].

2. Index of a Pair of Projections and Trindex

In this section we recall the main properties of the index of a Fredholm pair of orthogonal projections in $\mathcal{H}$ and discuss a closely related notion of a trindex of a pair of operators, one of which is a bounded operator in $\mathcal{H}$ and the other is an orthogonal projection in $\mathcal{H}$. Finally, we introduce the notion of a generalized trace for a pair of bounded operators in $\mathcal{H}$.

Let P and Q be orthogonal projections in a complex separable Hilbert space $\mathcal{H}$. The pair (P, Q) is said to be a Fredholm pair if the map

$$QP\big|_{\mathrm{ran}(P)} : \mathrm{ran}(P) \to \mathrm{ran}(Q) \tag{2.1}$$

is a Fredholm operator from the Hilbert space $\mathrm{ran}(P)$ to the Hilbert space $\mathrm{ran}(Q)$. In this case one defines the index of the pair (P, Q) as the Fredholm index of the operator $QP\big|_{\mathrm{ran}(P)}$

$$\mathrm{index}(P, Q) = \mathrm{index}(QP\big|_{\mathrm{ran}(P)}). \tag{2.2}$$

The following three results, Lemmas 2.1 and 2.3 and Theorem 2.2, recall well-known results for Fredholm pairs of projections. We refer, for instance, to [1], [3], [24], [25] and the references cited therein.

We start with two important criteria for a pair (P, Q) of self-adjoint projections to be a Fredholm pair.

Lemma 2.1. *(i) A necessary and sufficient condition that (P, Q) be a Fredholm pair is that $P - Q = F + D$, where F, D are self-adjoint, $\|D\| < 1$, and F is a finite-rank operator.*
(ii) (P, Q) is a Fredholm pair if and only if $+1$ and -1 do not belong to the essential spectrum of $(P - Q)$

$$\pm 1 \notin \mathrm{ess.spec}(P - Q). \tag{2.3}$$

In this case $\ker(P - Q \pm I_{\mathcal{H}})$ are both finite dimensional and

$$\mathrm{index}(P, Q) = \dim(\ker(P - Q - I_{\mathcal{H}})) - \dim(\ker(P - Q + I_{\mathcal{H}})). \tag{2.4}$$

In particular, if either

$$(P - Q) \in \mathcal{B}_\infty(\mathcal{H}), \tag{2.5}$$

or

$$\|P - Q\| < 1, \tag{2.6}$$

then (P, Q) is a Fredholm pair.

The following result summarizes some of the most important properties of the index of a Fredholm pair of projections.

Theorem 2.2. *(i) Let (P, Q) be a Fredholm pair of projections in $\mathcal{H}$. Then so is (Q, P) and*

$$\mathrm{index}(P, Q) = -\mathrm{index}(Q, P). \tag{2.7}$$

(ii) Let (P, Q) and (Q, R) be Fredholm pairs in $\mathcal{H}$ and either $(P - Q) \in \mathcal{B}_\infty(\mathcal{H})$ or $(Q - R) \in \mathcal{B}_\infty(\mathcal{H})$. Then (P, R) is a Fredholm pair and one has the chain rule

$$\mathrm{index}(P, R) = \mathrm{index}(P, Q) + \mathrm{index}(Q, R). \tag{2.8}$$

(iii) If $\|P - Q\| < 1$ then

$$\mathrm{index}(P, Q) = 0. \tag{2.9}$$

(iv) If $(P - Q) \in \mathcal{B}_1(\mathcal{H})$ then

$$\mathrm{index}(P, Q) = \mathrm{tr}(P - Q). \tag{2.10}$$

As shown in [3], the compactness assumption in connection with (2.8) cannot be dropped in general.

Theorem 2.2 (ii) combined with Lemma 2.1 (i) implies a stability result for the index for a Fredholm pair of projections under small perturbations.

Lemma 2.3. *Let P, P_1, and Q be orthogonal projections in $\mathcal{H}$. Assume that*

$$(P-Q) \in \mathcal{B}_\infty(\mathcal{H}) \tag{2.11}$$

and

$$\|P-P_1\| < 1. \tag{2.12}$$

Then (P,Q) and (P_1,Q) are Fredholm pairs in $\mathcal{H}$ and

$$\operatorname{index}(P,Q) = \operatorname{index}(P_1,Q). \tag{2.13}$$

Proof. That (P,Q) is a Fredholm pair follows from (2.11) and Lemma 2.1 (ii). Since (2.11) and (2.12) hold, the difference $P_1 - Q$ can be represented as a sum of a contraction (with norm strictly less than one) and a finite-rank operator. Thus (P_1,Q) is a Fredholm pair by Lemma 2.1 (i). Since (2.11) holds one can apply Theorem 2.2 (ii) to conclude that

$$\operatorname{index}(P,P_1) = \operatorname{index}(P,Q) + \operatorname{index}(Q,P_1). \tag{2.14}$$

By Theorem 2.2 (iii) and (2.12) one gets

$$\operatorname{index}(P,P_1) = 0. \tag{2.15}$$

Combining (2.7), (2.14), and (2.15) one arrives at (2.13). □

Definition 2.4. Let $A \in \mathcal{B}(\mathcal{H})$ and Q be an orthogonal projection in $\mathcal{H}$. We say that the pair (A,Q) has a *trindex*, denoted by $\operatorname{trindex}(A,Q)$, if there exists an orthogonal projection P in $\mathcal{H}$ such that $(A-P) \in \mathcal{B}_1(\mathcal{H})$ and (P,Q) is a Fredholm pair of orthogonal projections in $\mathcal{H}$. In this case the trindex of the pair (A,Q) is defined by

$$\operatorname{trindex}(A,Q) = \operatorname{tr}(A-P) + \operatorname{index}(P,Q). \tag{2.16}$$

The following result shows that the trindex of the pair (A,Q) is well-defined, that is, it is independent of the choice of the projection P satisfying the conditions in Definition 2.4.

Lemma 2.5. *Let $A \in \mathcal{B}(\mathcal{H})$, and P_1, P_2, and Q be orthogonal projections in $\mathcal{H}$ such that*

$$(A-P_j) \in \mathcal{B}_1(\mathcal{H}), \quad j=1,2, \tag{2.17}$$

and

$$(P_j,Q) \text{ is a Fredholm pair}, \quad j=1,2. \tag{2.18}$$

Then

$$\operatorname{tr}(A-P_1) + \operatorname{index}(P_1,Q) = \operatorname{tr}(A-P_2) + \operatorname{index}(P_2,Q). \tag{2.19}$$

Proof. By (2.17) one concludes that $(P_1-P_2) \in \mathcal{B}_1(\mathcal{H})$ and hence by Lemma 2.1 (ii), the pair (P_1,P_2) is a Fredholm pair. In particular, Theorem 2.2 (iv) implies

$$\operatorname{tr}(A-P_1) = \operatorname{tr}(A-P_2) + \operatorname{tr}(P_2-P_1) = \operatorname{tr}(A-P_2) + \operatorname{index}(P_2,P_1). \tag{2.20}$$

Hence, Theorem 2.2 (ii) yields

$$\begin{aligned} &\operatorname{tr}(A-P_1)+\operatorname{index}(P_1,Q)=\operatorname{tr}(A-P_2)+\operatorname{index}(P_2,P_1)+\operatorname{index}(P_1,Q)\\ &=\operatorname{tr}(A-P_2)+\operatorname{index}(P_2,Q) \end{aligned} \tag{2.21}$$

proving (2.19). □

Remark 2.6. Our motivation for introducing the concept of a trindex for a pair (A,Q) lies in the following two facts.
(i) If $A=P$, with (P,Q) a Fredholm pair of projections in $\mathcal{H}$, then

$$\operatorname{trindex}(P,Q)=\operatorname{index}(P,Q). \tag{2.22}$$

(ii) If $A\in\mathcal{B}(\mathcal{H})$ and Q is an orthogonal projection in $\mathcal{H}$ with $(A-Q)\in\mathcal{B}_1(\mathcal{H})$, then

$$\operatorname{trindex}(A,Q)=\operatorname{tr}(A-Q). \tag{2.23}$$

The stability result for the trindex of a pair (A,Q) analogous to Lemma 2.3 then reads as follows.

Lemma 2.7. *Let $A\in\mathcal{B}(\mathcal{H})$, and Q, Q_1 be orthogonal projections in $\mathcal{H}$ such that $(Q-Q_1)\in\mathcal{B}_\infty(\mathcal{H})$ and*

$$\|Q-Q_1\|<1. \tag{2.24}$$

If (A,Q) has a trindex, then (A,Q_1) has a trindex and

$$\operatorname{trindex}(A,Q)=\operatorname{trindex}(A,Q_1). \tag{2.25}$$

Proof. It suffices to combine Lemma 2.3 and (2.16). □

Definition 2.8. Let $A,B\in\mathcal{B}(\mathcal{H})$ and $(A-B)\in\mathcal{B}_\infty(\mathcal{H})$. We say that the pair (A,B) has a *generalized trace,* denoted by $\operatorname{gtr}(A,B)$, if there exists an orthogonal projection Q in $\mathcal{H}$ such that both pairs, (A,Q) and (B,Q) have a trindex. In this case the generalized trace of the pair (A,B) is defined by

$$\operatorname{gtr}(A,B)=\operatorname{trindex}(A,Q)-\operatorname{trindex}(B,Q). \tag{2.26}$$

The following result shows that $\operatorname{gtr}(A,B)$ is well-defined, that is, it is independent of the choice of the orthogonal projection Q satisfying the conditions in Definition 2.8.

Lemma 2.9. *Let $A,B\in\mathcal{B}(\mathcal{H})$, $(A-B)\in\mathcal{B}_\infty(\mathcal{H})$, and Q_1,Q_2 orthogonal projections in $\mathcal{H}$ such that (A,Q_j) and (B,Q_j), $j=1,2$ have a trindex. Then*

$$\operatorname{trindex}(A,Q_1)-\operatorname{trindex}(B,Q_1)=\operatorname{trindex}(A,Q_2)-\operatorname{trindex}(B,Q_2). \tag{2.27}$$

Proof. By hypothesis, there exist orthogonal projections $P_{j,A},P_{j,B}$ in $\mathcal{H}$ such that $(A-P_{j,A}),(B-P_{j,B})\in\mathcal{B}_1(\mathcal{H})$ and the pairs $(P_{j,A},Q_j)$ and $(P_{j,B},Q_j)$, $j=1,2$ are Fredholm pairs of projections. Since $(A-B)\in\mathcal{B}_\infty(\mathcal{H})$ one infers $(P_{j,A}-P_{k,B})\in\mathcal{B}_\infty(\mathcal{H})$, $j,k\in\{1,2\}$ and hence $(P_{j,A},P_{k,B})$, $j,k\in\{1,2\}$ are Fredholm pairs. Moreover, $(P_{2,A}-P_{1,A}),(P_{2,B}-P_{1,B})\in\mathcal{B}_1(\mathcal{H})$. Thus,

$$\begin{aligned} &\operatorname{trindex}(A,Q_1)-\operatorname{trindex}(B,Q_1)-(\operatorname{trindex}(A,Q_2)-\operatorname{trindex}(B,Q_2))\\ &=\operatorname{tr}(A-P_{1,A})+\operatorname{index}(P_{1,A},Q_1)-\operatorname{tr}(A-P_{2,A})-\operatorname{index}(P_{2,A},Q_2)\\ &-\operatorname{tr}(B-P_{1,B})-\operatorname{index}(P_{1,B},Q_1)+\operatorname{tr}(B-P_{2,B})+\operatorname{index}(P_{2,B},Q_2)\\ &=\operatorname{tr}((A-B-P_{1,A}+P_{1,B})-(A-B-P_{2,A}+P_{2,B}))+\operatorname{index}(P_{1,A},Q_1) \end{aligned}$$

$$\begin{aligned}
&- \operatorname{index}(P_{1,B}, Q_1) + \operatorname{index}(P_{2,B}, Q_2) - \operatorname{index}(P_{2,A}, Q_2)\\
&= \operatorname{tr}(P_{2,A} - P_{1,A}) - \operatorname{tr}(P_{2,B} - P_{1,B}) + \operatorname{index}(P_{1,A}, P_{1,B}) + \operatorname{index}(P_{2,B}, P_{2,A})\\
&= \operatorname{index}(P_{2,A}, P_{1,A}) + \operatorname{index}(P_{1,A}, P_{1,B}) - \operatorname{index}(P_{2,B}, P_{1,B}) + \operatorname{index}(P_{2,B}, P_{2,A})\\
&= \operatorname{index}(P_{2,A}, P_{1,B}) + \operatorname{index}(P_{1,B}, P_{2,A}) = 0 \qquad (2.28)
\end{aligned}$$

by repeatedly using (2.7) and (2.8). □

Remark 2.10. If $A, B \in \mathcal{B}(\mathcal{H})$ with $(A - B) \in \mathcal{B}_1(\mathcal{H})$, then

$$\operatorname{gtr}(A, B) = \operatorname{tr}(A - B). \tag{2.29}$$

We were somewhat hesitant to introduce concepts such as *trindex*, $\operatorname{trindex}(\cdot,\cdot)$ and *generalized trace*, $\operatorname{gtr}(\cdot,\cdot)$ as additional entities to such familiar quantities like the Fredholm index, $\operatorname{index}(\cdot,\cdot)$ and the trace, $\operatorname{tr}(\cdot)$. However, it will become clear from the remainder of this paper, that both objects seem to be very natural in the context of Krein's spectral shift function (cf. Corollary 3.10 and Remark 5.4).

3. The Ξ Operator

Suppose T is a bounded dissipative operator in the Hilbert space $\mathcal{H}$ (i.e., $\operatorname{Im}(T) \geq 0$) and L is the minimal self-adjoint dilation of T (cf. [52, Ch. III]) in the Hilbert space $\mathcal{K} \supseteq \mathcal{H}$. We define the Ξ-operator associated with the dissipative operator T by

$$\Xi(T) = P_{\mathcal{H}} E_L((-\infty, 0)) P_{\mathcal{H}}|_{\mathcal{H}}, \tag{3.1}$$

where $P_{\mathcal{H}}$ is the orthogonal projection in $\mathcal{K}$ onto $\mathcal{H}$ and $\{E_L(\lambda)\}_{\lambda\in\mathbb{R}}$ represents the family of strongly right-continuous orthogonal spectral projections of L in $\mathcal{K}$.

In particular, if $T = T^*$, the Ξ-operator coincides with the spectral projection of T corresponding to the negative semi-axis $(-\infty, 0)$,

$$\Xi(T) = E_T((-\infty, 0)), \tag{3.2}$$

since in this case the minimal self-adjoint dilation of T coincides with T.

Remark 3.1. (i) By (3.1), Ξ is a nonnegative contraction,

$$0 \leq \Xi(T) \leq I_{\mathcal{H}}. \tag{3.3}$$

(ii) If $T \in \mathcal{B}(\mathcal{H})$ is a bounded dissipative operator and $T^{-1} \in \mathcal{B}(\mathcal{H})$ then $\Xi(T)$ can be expressed in terms of the operator logarithm of T by

$$\Xi(T) = \pi^{-1} \operatorname{Im}(\log(T)), \tag{3.4}$$

where $\log(T)$ is defined by

$$\log(T) = -i \int_0^\infty d\lambda\, ((T + i\lambda)^{-1} - (1 + i\lambda)^{-1} I_{\mathcal{H}}) \tag{3.5}$$

in the sense of a $\mathcal{B}(\mathcal{H})$-norm convergent Riemann integral (cf. the extensive treatment in [19]). Without going into details (these may be found in [19]), we remark that (3.4) resembles the exponential Herglotz representation for scalar-valued Herglotz functions studied in detail by Aronszajn and Donoghue [2]. Indeed, for any Herglotz function $t(z)$ (i.e., $t : \mathbb{C}_+ \to \mathbb{C}_+$ analytically), $\log(t(z))$ is also a Herglotz function admitting the representation,

$$\log(t(z)) = c + \int_{\mathbb{R}} d\lambda\, \xi(\lambda)((\lambda - z)^{-1} - \lambda(1 + \lambda^2)^{-1}), \quad z \in \mathbb{C}_+, \tag{3.6}$$

where $c \in \mathbb{R}$ and

$$0 \le \xi \le 1 \text{ and } \xi(\lambda) = \pi^{-1} \lim_{\varepsilon \downarrow 0} \operatorname{Im}(\log(t(\lambda + i\varepsilon))) \text{ a.e.} \tag{3.7}$$

At this point a natural question arises. Suppose S is a bounded dissipative operator in $\mathcal{H}$ and $T = S + A + iB$, $A = A^* \in \mathcal{B}(\mathcal{H})$, $0 \le B \in \mathcal{B}(\mathcal{H})$ its dissipative bounded perturbation. Can one expect an interesting relationship between $\Xi(T)$ and $\Xi(S)$? The following is a first result in this direction.

Lemma 3.2. *Let $S, T \in \mathcal{B}(\mathcal{H})$ be dissipative operators such that $S^{-1}, T^{-1} \in \mathcal{B}(\mathcal{H})$ and assume $(T - S) \in \mathcal{B}_1(\mathcal{H})$. Then*

$$(\Xi(T) - \Xi(S)) \in \mathcal{B}_1(\mathcal{H}). \tag{3.8}$$

Proof. Since S and T have a bounded inverse, $\log(T)$ and $\log(S)$ are well-defined and (cf. [19])

$$\begin{aligned} \log(T) - \log(S) &= -i \int_0^\infty dt\, ((T + it)^{-1} - (S + it)^{-1}) \\ &= i \int_0^\infty dt\, ((T + it)^{-1}(T - S)(S + it)^{-1}). \end{aligned} \tag{3.9}$$

Using standard estimates for resolvents $(T + it)^{-1}$ and $(S + it)^{-1}$ $(t \ge 0)$ of the dissipative operators T and S entering (3.9) (cf. Lemma 2.6 in [19]) one concludes

$$(\log(T) - \log(S)) \in \mathcal{B}_1(\mathcal{H}), \tag{3.10}$$

if $(T - S) \in \mathcal{B}_1(\mathcal{H})$. Thus, $(\Xi(T) - \Xi(S)) \in \mathcal{B}_1(\mathcal{H})$ by (3.4) and (3.10). $\square$

We assume the following hypothesis in the sequel.

Hypothesis 3.3. *Assume $S = S^* \in \mathcal{B}(\mathcal{H})$, $A = A^* \in \mathcal{B}_\infty(\mathcal{H})$, $0 \le B \in \mathcal{B}_1(\mathcal{H})$, and $(S + A + \tau_0 B)^{-1} \in \mathcal{B}(\mathcal{H})$ for some $\tau_0 \in \mathbb{R}$.*

Remark 3.4. Under Hypothesis 3.3 one infers

$$0 \notin \text{ess.spec}(S) \tag{3.11}$$

by the stability of the essential spectrum under compact perturbations. Moreover, by the analytic Fredholm theorem (cf. [43, Sect. VI.5]), $(S+A+zB)^{-1} \in \mathcal{B}(\mathcal{H})$, $z \in \overline{\mathbb{C}_+}$ except for z in a discrete set $\mathcal{D} \subset \mathbb{R}$, with $\pm\infty$ the only possible accumulation points of $\mathcal{D}$. In particular,

$$(S + A + \varepsilon B)^{-1} \in \mathcal{B}(\mathcal{H}) \text{ for } \varepsilon \text{ sufficiently small, } \varepsilon \ne 0. \tag{3.12}$$

Lemma 3.5. *Assume Hypothesis* 3.3 *with $A = 0$. Then*

$$(\Xi(S + tB) - \Xi(S)) \in \mathcal{B}_1(\mathcal{H}) \text{ for all } t \in \mathbb{R} \tag{3.13}$$

and

$$\|\Xi(S + tB) - \Xi(S)\|_{\mathcal{B}_1(\mathcal{H})} = O(t) \text{ as } t \downarrow 0. \tag{3.14}$$

Moreover, $S + zB$, $z \in \mathbb{C}_+$ has a bounded inverse,

$$(S + zB)^{-1} \in \mathcal{B}(\mathcal{H}) \text{ for all } z \in \mathbb{C}_+ \tag{3.15}$$

and

$$(\Xi(S + zB) - \Xi(S)) \in \mathcal{B}_1(\mathcal{H}) \text{ for all } z \in \overline{\mathbb{C}_+}\,. \tag{3.16}$$

Proof. Since $(S+\tau_0 B)^{-1} \in \mathcal{B}(\mathcal{H})$ for some $\tau_0 \in \mathbb{R}$ and $B \in \mathcal{B}_\infty(\mathcal{H})$, one infers that $0 \notin \text{ess.spec}(S)$. Thus, there exists a closed interval Δ, $0 \in \Delta$, such that $\dim(\text{ran}(E_{S+tB}(\Delta))) < \infty$ for all $t \in \mathbb{R}$. Hence, for given $t \in \mathbb{R}$, one can find a clockwise oriented bounded contour Γ_t encircling $(\text{spec}(S+tB) \cup \text{spec}(S)) \cap (-\infty, 0)$ such that

$$\Xi(S+tB) = E_{S+tB}((-\infty,0)) = \frac{1}{2\pi i}\oint_{\Gamma_t} d\zeta\, (S+tB-\zeta)^{-1}, \quad t \in \mathbb{R} \tag{3.17}$$

and

$$\Xi(S) = E_S((-\infty,0)) = \frac{1}{2\pi i}\oint_{\Gamma_t} d\zeta\, (S-\zeta)^{-1}. \tag{3.18}$$

The second resolvent identity for $S+tB$ and S then implies $((S+tB-\zeta)^{-1} - (S-\zeta)^{-1}) \in \mathcal{B}_1(\mathcal{H})$, $\zeta \in \Gamma_t$, proving (3.13).

Since $B \geq 0$, there exists a closed interval Δ, $\Delta \subset (-\infty, 0)$, such that

$$\bigcup_{t\in[0,\varepsilon]} \text{spec}(S+tB) \cap (-\infty,0) \subset \Delta \text{ for } \varepsilon > 0 \text{ sufficiently small.} \tag{3.19}$$

Thus, choosing the contour

$$\Gamma = \{\zeta \in \mathbb{C} \,|\, \text{dist}(\zeta,\Delta) = \frac{1}{2}\text{dist}(0,\Delta)\}, \tag{3.20}$$

the representation (3.17) is valid for all $t \in [0,\varepsilon]$, for sufficiently small $\varepsilon > 0$. Using the second resolvent identity again and the standard estimate $\|(A-\zeta)^{-1}\| \leq (\text{dist}(\zeta, \text{spec}(A)))^{-1}$ for every self-adjoint operator A in $\mathcal{H}$, one obtains

$$\begin{aligned} \|\Xi(S+tB) - \Xi(S)\|_{\mathcal{B}_1(\mathcal{H})} &= \|E_{S+tB}((-\infty,0)) - E_S((-\infty,0))\|_{\mathcal{B}_1(\mathcal{H})} \\ &\leq (2/\pi)t(\text{dist}(0,\Delta))^{-2}\|B\|_{\mathcal{B}_1(\mathcal{H})}|\Gamma|, \quad t \in [0,\varepsilon], \end{aligned} \tag{3.21}$$

where $|\Gamma|$ denotes the length of the contour Γ. This proves (3.14).

Next, consider the operator-valued Herglotz function

$$M(z) = S + zB, \quad z \in \mathbb{C}_+ \tag{3.22}$$

(i.e., $\text{Im}(M(z)) \geq 0$ for all $z \in \mathbb{C}_+$). By hypothesis there exists a $\tau_0 \in \mathbb{R}$ such that $(S+\tau_0 B)^{-1} \in \mathcal{B}(\mathcal{H})$. Thus, for sufficiently small values of $|z-\tau_0|$, $z \in \mathbb{C}_+$, the operator $M(z)$, being a small perturbation of the invertible operator $S+\tau_0 B$, has a bounded inverse. By Lemma 2.3 in [19] and (3.13), $M(z)$ is invertible for all $z \in \mathbb{C}_+$, proving (3.15).

Since $S + zB$, $z \in \mathbb{C}_+$, and $S+\tau_0 B$ are boundedly invertible (dissipative) operators, Lemma 3.2 implies $(\Xi(S+zB) - \Xi(S+\tau_0 B)) \in \mathcal{B}_1(\mathcal{H})$. By (3.13), $(\Xi(S+\tau_0 B) - \Xi(S)) \in \mathcal{B}_1(\mathcal{H})$ implying (3.16). ☐

Remark 3.6. We note that condition (3.11) is crucial in connection with (3.13). Indeed, there exists $S = S^* \in \mathcal{B}(\mathcal{H})$ with $0 \in \text{ess.spec}(S)$ and a self-adjoint rank-one operator B, such that

$$\Xi(S+B) - \Xi(S) = E_{S+B}((-\infty,0)) - E_S((-\infty,0)) \notin \mathcal{B}_1(\mathcal{H}) \tag{3.23}$$

as implied by a result of Krein [30].

Corollary 3.7. *Assume the hypotheses of Lemma* 3.5*. Then*

$$\text{tr}(\Xi(S+tB) - \Xi(S)) = 0 \textit{ for } t > 0 \textit{ sufficiently small} \tag{3.24}$$

and

$$\operatorname{tr}(\Xi(S-tB)-\Xi(S)) = \dim(\ker(S)) \text{ for } t>0 \text{ sufficiently small.} \tag{3.25}$$

Proof. Eq. (3.24) follows from (3.14) and Theorem 2.2 (iii),(iv). Next one notes that for $t>0$ sufficiently small, $E_{S-tB}(\{0\})=0$ by Remark 3.4, and hence

$$\begin{aligned}
\Xi(S-tB)-\Xi(S) &= E_{S-tB}((-\infty,0)) - E_S((-\infty,0)) \\
&= E_S([0,\infty)) - E_{S-tB}([0,\infty)) = E_S([0,\infty)) - E_{S-tB}((0,\infty)) \\
&= E_S(\{0\}) + E_S((0,\infty)) - E_{S-tB}((0,\infty)) \\
&= E_S(\{0\}) + E_{-S}((-\infty,0)) - E_{-S+tB}((-\infty,0)) \\
&= E_S(\{0\}) + \Xi(-S) - \Xi(-S+tB).
\end{aligned} \tag{3.26}$$

Since by (3.24) (replacing S by $-S$),

$$\operatorname{tr}(\Xi(-S)-\Xi(-S+tB)) = 0 \text{ for sufficiently small } t>0, \tag{3.27}$$

one obtains (3.25). □

Lemma 3.2 yields $(\Xi(T)-\Xi(S)) \in \mathcal{B}_1(\mathcal{H})$ for $S=S^* \in \mathcal{B}(\mathcal{H})$ and T a dissipative operator with $(T-S)\in\mathcal{B}_1(\mathcal{H})$.

In the case of general compact perturbations with trace class imaginary parts, Hypothesis 3.3 is not sufficient for the difference $(\Xi(S+A+iB)-\Xi(S))$ to be of trace class (see Remark 3.11 below). The following result, however, shows that the pair $(\Xi(S+A+iB),\Xi(S))$ has a trindex.

Lemma 3.8. *Assume Hypothesis* 3.3*. Then*

$$(\Xi(S+A+iB)-\Xi(S+A)) \in \mathcal{B}_1(\mathcal{H}) \tag{3.28}$$

and the pair $(\Xi(S+A),\Xi(S))$ is a Fredholm pair of orthogonal projections. Thus, $(\Xi(S+A+iB),\Xi(S))$ has a trindex and

$$\begin{aligned}
&\operatorname{trindex}(\Xi(S+A+iB),\Xi(S)) \\
&\quad = \operatorname{tr}(\Xi(S+A+iB)-\Xi(S+A))) + \operatorname{index}(\Xi(S+A),\Xi(S)).
\end{aligned} \tag{3.29}$$

Proof. Since by hypothesis $(S+A+\tau_0 B)^{-1}\in\mathcal{B}(\mathcal{H})$ for some $\tau_0\in\mathbb{R}$, (3.16) implies (3.28). Due to the fact that $0\notin \operatorname{ess.spec}(S)$ (cf. Remark 3.4) one can represent the spectral projections $\Xi(S+A)=E_{S+A}((-\infty,0))$ and $\Xi(S)=E_S((-\infty,0))$ by the Riesz integrals (3.17), (3.18) and arguing as in the proof of Lemma 3.5 then yields

$$(\Xi(S+A)-\Xi(S))\in\mathcal{B}_\infty(\mathcal{H}). \tag{3.30}$$

Thus, by Lemma 2.1 (ii), the pair $(\Xi(S+A),\Xi(S))$ is a Fredholm pair of orthogonal projections, which together with (3.28) proves (3.29). □

Lemma 3.9. *Let S be a signature operator, that is, $S=S^*=S^{-1}$ and $A=A^*\in\mathcal{B}_2(\mathcal{H})$. Then*

$$(\Xi(S+A)-\Xi(S))\in\mathcal{B}_1(\mathcal{H}) \tag{3.31}$$

if and only if

$$[A,S]=(AS-SA)\in\mathcal{B}_1(\mathcal{H}). \tag{3.32}$$

Proof. Define two orthogonal projections $P = S_+$ and $Q = S_-$ such that $P+Q = I_{\mathcal{H}}$ and $S = P - Q$, where $S_\pm = (|S| \pm S)/2$ (taking into account that $\ker(S) = \{0\}$). Next, we note

$$\begin{aligned}
&\frac{1}{2\pi i}\oint_\Gamma d\zeta (S-\zeta)^{-1}A(S-\zeta)^{-1}\\
&= PAP\frac{1}{2\pi i}\oint_\Gamma d\zeta(1-\zeta)^{-2} + QAQ\frac{1}{2\pi i}\oint_\Gamma d\zeta(-1-\zeta)^{-2}\\
&+ (PAQ+QAP)\frac{1}{2\pi i}\oint_\Gamma d\zeta(1-\zeta)^{-1}(-1-\zeta)^{-1} = \frac{1}{4}S[S,A],
\end{aligned} \tag{3.33}$$

where the clockwise oriented contour Γ encircles $\operatorname{spec}(S+A)\cap(-\infty,0)$. On the other hand,

$$\begin{aligned}
&\Xi(S+A) - \Xi(S) = E_{S+A}((-\infty,0)) - E_S((-\infty,0))\\
&= -\frac{1}{2\pi i}\oint_\Gamma d\zeta(S-\zeta)^{-1}A(S-\zeta)^{-1}\\
&\quad + \frac{1}{2\pi i}\oint_\Gamma d\zeta(S+A-\zeta)^{-1}A(S-\zeta)^{-1}A(S-\zeta)^{-1}\\
&= -\frac{1}{4}S[S,A] + \frac{1}{2\pi i}\oint_\Gamma d\zeta(S+A-\zeta)^{-1}A(S-\zeta)^{-1}A(S-\zeta)^{-1}
\end{aligned} \tag{3.34}$$

using (3.33). Since $A \in \mathcal{B}_2(\mathcal{H})$, the last term in (3.34) is a trace class operator and, hence, $(\Xi(S+A) - \Xi(S)) \in \mathcal{B}_1(\mathcal{H})$ if and only if $[S,A] \in \mathcal{B}_1(\mathcal{H})$. □

Combining the results of Lemmas 3.8 and 3.9 we get the following result.

Corollary 3.10. *Assume $A = A^* \in \mathcal{B}_2(\mathcal{H})$, $0 \le B \in \mathcal{B}_1(\mathcal{H})$, and $S = S^* = S^{-1}$. Then*

$$(\Xi(S+A+iB) - \Xi(S)) \in \mathcal{B}_1(\mathcal{H}) \tag{3.35}$$

if and only if

$$[A,S] \in \mathcal{B}_1(\mathcal{H}). \tag{3.36}$$

Remark 3.11. Corollary 3.10 illustrates why Hypothesis 3.3 is insufficient to garantee (3.35). Indeed, choosing $\mathcal{H} = \mathcal{K}\oplus\mathcal{K}$, $S = I_{\mathcal{K}} \oplus (-I_{\mathcal{K}})$, and $A = \left(\begin{smallmatrix} 0 & a \\ a & 0\end{smallmatrix}\right)$, where $a \in \mathcal{B}_2(\mathcal{K})\backslash\mathcal{B}_1(\mathcal{K})$ with $||a|| < 1/2$ for some (necessarily infinite dimensional) complex separable Hilbert space $\mathcal{K}$, one infers the tripple (S,A,B) satisfies Hypothesis 3.3 for any $0 \le B \in \mathcal{B}_1(\mathcal{H})$ and $[A,S] \notin \mathcal{B}_1(\mathcal{H})$. Consequently, in this case,

$$(\Xi(S+A+iB) - \Xi(S)) \notin \mathcal{B}_1(\mathcal{H}) \tag{3.37}$$

by Corollary 3.10.

The next result concerns the continuity of $\operatorname{trindex}(\Xi(S+A+iB),\Xi(S))$ under small perturbations of A and B in the operator and trace norm topology, respectively.

Theorem 3.12. *Assume Hypothesis* 3.3. *Let $A_j = A_j^* \in \mathcal{B}_\infty(\mathcal{H})$, $0 \le B_j \in \mathcal{B}_1(\mathcal{H})$, $j \in \mathbb{N}$, such that $\lim_{j\to\infty}||A_j - A|| = 0$ and $\lim_{j\to\infty}||B_j - B||_{\mathcal{B}_1(\mathcal{H})} = 0$. Then*

$$\lim_{j\to\infty} \operatorname{trindex}(\Xi(S+A_j+iB_j),\Xi(S))) = \operatorname{trindex}(\Xi(S+A+iB),\Xi(S))). \tag{3.38}$$

Proof. By hypothesis, $(S+A+\tau_0 B)^{-1} \in \mathcal{B}(\mathcal{H})$ for some $\tau_0 \in \mathbb{R}$. Since $\|A_j - A\| \to 0$ and $\|B_j - B\| \to 0$ as $j \to \infty$, the operators $S + A_j + \tau_0 B_j$ are also invertible for $j \geq j_0$, j_0 sufficiently large. Since the operator-valued logarithm is a continuous function of its (dissipative) argument in the $\mathcal{B}(\mathcal{H})$-topology,

$$\operatorname*{n-lim}_{j\to\infty} \log(S + A_j + \tau_0 B_j) = \log(S + A + \tau_0 B) \tag{3.39}$$

and hence by (3.4),

$$\operatorname*{n-lim}_{j\to\infty} \Xi(S + A_j + \tau_0 B_j) = \Xi(S + A + \tau_0 B). \tag{3.40}$$

By Remark 3.4, $0 \notin \text{ess.spec}(S)$ and thus

$$(\Xi(S + A_j + \tau_0 B_j) - \Xi(S)) \in \mathcal{B}_\infty(\mathcal{H}) \tag{3.41}$$

and

$$(\Xi(S + A + \tau_0 B) - \Xi(S)) \in \mathcal{B}_\infty(\mathcal{H}). \tag{3.42}$$

Thus the difference $(\Xi(S + A_j + \tau_0 B_j) - \Xi(S + A + \tau_0 B))$ is a compact operator and hence by (3.40) and Lemma 2.3 one gets

$$\lim_{j\to\infty} \operatorname{index}(\Xi(S + A_j + \tau_0 B_j), \Xi(S)) = \operatorname{index}(\Xi(S + A + \tau_0 B), \Xi(S))). \tag{3.43}$$

The estimate $(t \geq 0)$

$$\begin{aligned}
&\|(S + A + iB + it)^{-1} - (S + A + \tau_0 B + it)^{-1} \\
&- (S + A_j + iB_j + it)^{-1} + (S + A_j + \tau_0 B_j + it)^{-1}\|_{\mathcal{B}_1(\mathcal{H})} \\
&= (1 + t^2)^{-1} o(1) \text{ as } j \to \infty,
\end{aligned} \tag{3.44}$$

with remainder term $o(1)$ uniform with respect to $t \geq 0$, then yields

$$\begin{aligned}
\lim_{j\to\infty} &\| \log(S + A_j + iB_j) - \log(S + A_j + \tau_0 B_j) \\
&- \log(S + A + iB) - \log(S + A + \tau_0 B)\|_{\mathcal{B}_1(\mathcal{H})} = 0.
\end{aligned} \tag{3.45}$$

Hence

$$\begin{aligned}
\lim_{j\to\infty} &\|\Xi(S + A_j + iB_j) - \Xi(S + A_j + \tau_0 B_j) \\
&- \Xi(S + A + iB) + \Xi(S + A + \tau_0 B)\|_{\mathcal{B}_1(\mathcal{H})} = 0.
\end{aligned} \tag{3.46}$$

Combining (3.43) and (3.46) yields

$$\begin{aligned}
&\lim_{j\to\infty} (\operatorname{tr}(\Xi(S + A_j + iB_j) - \Xi(S + A_j + \tau_0 B_j)) + \operatorname{index}(\Xi(S + A_j + \tau_0 B_j), \Xi(S))) \\
&\quad = \operatorname{tr}(\Xi(S + A + iB) - \Xi(S + A + \tau_0 B)) + \operatorname{index}(\Xi(S + A + \tau_0 B), \Xi(S)) \\
&\quad = \operatorname{trindex}(\Xi(S + A + iB), \Xi(S)),
\end{aligned} \tag{3.47}$$

proving (3.38). ∎

4. Averaged Fredholm Indices and the Birman–Krein Formula

Assume Hypothesis 3.3 with $A = 0$. By Remark 3.4 the operators $S + zB$, $z \in \mathbb{C}$ have a bounded inverse except for z in a discrete set $\mathcal{D} \subset \mathbb{R}$ with $\pm\infty$ the only possible accumulation points of $\mathcal{D}$. Introducing the family of normal trace class operators

$$\mathcal{A}(z) = B^{1/2}(S + zB)^{-1}B^{1/2}, \quad z \in \mathbb{C}\backslash\mathcal{D}. \tag{4.1}$$

one verifies the resolvent-type identities

$$\mathcal{A}(z_1) - \mathcal{A}(z_2) = (z_2 - z_1)\mathcal{A}(z_1)\mathcal{A}(z_2), \quad \frac{d}{dz}\mathcal{A}(z) = -\mathcal{A}(z)^2. \tag{4.2}$$

Thus, $\mathcal{A}(z_1)$ and $\mathcal{A}(z_2)$ commute for all $z_1, z_2 \in \mathbb{C}\backslash\mathcal{D}$ and have a common complete orthogonal system of eigenvectors, denoted by $\{\varphi_k\}_{k=1}^\infty$.

Making use of (4.2) one immediately gets the following result.

Lemma 4.1. *The operator $\mathcal{A}(z)$, $z \in \mathbb{C}\backslash\mathcal{D}$ has the eigenvalue z^{-1} with multiplicity $\dim(\ker(S))$. In particular, if $S^{-1} \in \mathcal{B}(\mathcal{H})$, then*

$$z^{-1} \notin \operatorname{spec}(\mathcal{A}(z)). \tag{4.3}$$

Let φ be an eigenvector of $\mathcal{A}(z_1)$ corresponding to the eigenvalue $\mu(z_1)$. Then φ is an eigenvector of $\mathcal{A}(z_2)$ corresponding to the eigenvalue

$$\mu(z_2) = \frac{\mu(z_1)}{1 - \mu(z_1)(z_1 - z_2)} \tag{4.4}$$

of the same multiplicity and,

$$1 - \mu(z_1)(z_1 - z_2) \neq 0. \tag{4.5}$$

Under Hypothesis 3.3 with $A = 0$, the operator $\mathcal{A}(\varepsilon)$ is well-defined for small (real) values of ε, $\varepsilon \neq 0$, $\mathcal{A}(\varepsilon) \in \mathcal{B}_1(\mathcal{H})$ (cf. Remark 3.4) and hence $\arctan(\mathcal{A}(\varepsilon)) \in \mathcal{B}_1(\mathcal{H})$.

Theorem 4.2. *Assume Hypothesis* 3.3 *with $A = 0$. Then*

$$\lim_{\varepsilon\downarrow 0} \operatorname{tr}(\arctan(\mathcal{A}(\varepsilon))) = \int_{\mathbb{R}} \frac{dt\, n^*(t)}{1 + t^2}, \tag{4.6}$$

where $n^*(t)$ is the left-continuous function.

$$n^*(t) = \begin{cases} \sum_{s\in[0,t)} \dim(\ker(sB - S)), & t > 0, \\ 0, & t = 0, \\ -\sum_{s\in[t,0)} \dim(\ker(sB - S)), & t < 0. \end{cases} \tag{4.7}$$

Proof. Fix a $\delta_0 \in \mathbb{R}$, $\delta_0 \notin \mathcal{D}$. Denote by $\{\mu_k(\delta_0)\}_{k\in\mathbb{N}} \subset \operatorname{spec}(\mathcal{A}(\delta_0))\backslash\{\delta_0^{-1}\}$ the eigenvalues of $\mathcal{A}(\delta_0)$ different from δ_0^{-1} with corresponding multiplicities $\{m_k\}_{k\in\mathbb{N}}$. First we prove the following representation,

$$\lim_{\varepsilon\downarrow 0} \operatorname{tr}(\arctan(\mathcal{A}(\varepsilon))) = \sum_{k=1}^\infty m_k \arctan(\lambda_k) + \frac{\pi}{2}\dim(\ker(S)), \tag{4.8}$$

with

$$\lambda_k = \frac{\mu_k(\delta_0)}{1 - \mu_k(\delta_0)\delta_0}, \quad k \in \mathbb{N}. \tag{4.9}$$

Since $\mathcal{A}(\delta_0) \in \mathcal{B}_\infty(\mathcal{H})$, there exists a $\gamma > 0$ such that

$$\operatorname{spec}(\mathcal{A}(\delta_0)) \cap (\delta_0^{-1} - \gamma, \delta_0^{-1} + \gamma) = \begin{cases} \emptyset, & \dim(\ker(S)) = 0, \\ \{\delta_0^{-1}\}, & \dim(\ker(S)) > 0. \end{cases} \tag{4.10}$$

For sufficiently small values of $\varepsilon \in \mathbb{R}$, $\varepsilon \neq 0$, the self-adjoint operator $\mathcal{A}(\varepsilon)$ is well-defined and the trace of $\arctan(\mathcal{A}(\varepsilon))$ reads

$$\operatorname{tr}(\arctan(\mathcal{A}(\varepsilon))) = \sum_{k=1}^{\infty} m_k \arctan(\mu_k(\varepsilon)) + \dim(\ker(S)) \arctan(\varepsilon^{-1}), \tag{4.11}$$

where by Lemma 4.1,

$$\mu_k(\varepsilon) = \frac{\mu_k(\delta_0)}{1 - \mu_k(\delta_0)(\delta_0 - \varepsilon)}, \quad k \in \mathbb{N}. \tag{4.12}$$

For $\varepsilon < \frac{\gamma\delta_0}{2} \|\mathcal{A}(\delta_0)\|^{-1}$ one obtains

$$\begin{aligned} &\bigg| \sum_{k=1}^{\infty} m_k \arctan(\mu_k(\varepsilon)) - \sum_{k=1}^{\infty} m_k \arctan(\lambda_k) \bigg| \\ &\leq \sum_{k=1}^{\infty} m_k |\mu_k(\delta_0)| \, |(1 - \mu_k(\delta_0)\delta_0)^{-1} - (1 - \mu_k(\delta_0)(\delta_0 - \varepsilon))^{-1}| \\ &\leq 2\varepsilon(\gamma\delta_0)^{-2} \sum_{k=1}^{\infty} m_k |\mu_k(\delta_0)|^2 \leq 2\varepsilon(\gamma\delta_0)^{-2} \|\mathcal{A}(\delta_0)\|^2_{\mathcal{B}_2(\mathcal{H})}. \end{aligned} \tag{4.13}$$

By (4.13), using the dominated convergence theorem, one can perform the limit $\varepsilon \downarrow 0$ in (4.11) and upon combining (4.9) and (4.12) one arrives at (4.8) using Lemma 4.1.

Since the multiplicities $m_k = \dim(\ker(B^{1/2}(S + \delta_0 B)^{-1} B^{1/2} - \mu_k(\delta_0) I_{\mathcal{H}}))$ of the eigenvalues $\mu_k(\delta_0)$ can also be computed as

$$m_k = \dim(\ker(B - \lambda_k S)), \tag{4.14}$$

where λ_k are given by (4.9), the absolutely convergent series $\sum_{k=1}^{\infty} m_k \arctan(\lambda_k)$ can be represented as the Lebesgue integral

$$\sum_{k=1}^{\infty} m_k \arctan(\lambda_k) = \sum_{k=1}^{\infty} m_k \int_0^{\lambda_k} \frac{dt}{1+t^2} = \int_{\mathbb{R}} \frac{dt\, m(t)}{1+t^2}, \tag{4.15}$$

where $m(t)$ is the following eigenvalue counting function

$$m(t) = \begin{cases} \sum_{\lambda \in (t,\infty)} \dim(\ker(B - \lambda S)), & t > 0, \\ 0, & t = 0, \\ -\sum_{\lambda \in (-\infty,t)} \dim(\ker(B - \lambda S)), & t < 0. \end{cases} \tag{4.16}$$

Making the change of variables $t \to 1/t$ (separately on $(-\infty, 0)$ and $(0, \infty)$)

$$\int_{\mathbb{R}} \frac{dt\, m(t)}{1+t^2} = \int_{\mathbb{R}} \frac{dt\, m(1/t)}{1+t^2}, \tag{4.17}$$

one infers by (4.15) and (4.8) that

$$\lim_{\varepsilon \downarrow 0} \operatorname{tr}(\arctan(\mathcal{A}(\varepsilon))) = \int_{\mathbb{R}} \frac{dt\, m(1/t)}{1+t^2} + \dim(\ker(S)) \int_0^{\infty} \frac{dt}{1+t^2} = \int_{\mathbb{R}} \frac{dt\, n(t)}{1+t^2}, \tag{4.18}$$

where

$$n(t) = m(1/t) + \dim(\ker(S))\frac{1+\operatorname{sgn}(t)}{2}, \quad t \neq 0. \tag{4.19}$$

Combining (4.16) and (4.19) one concludes that $n(t) = n^*(t)$ for a.e. $t \in \mathbb{R}$, where $n^*(t)$ is a left-continuous function given by (4.7). ☐

The following result is one of the main technical tools in our paper.

Theorem 4.3. *Let $S = S^* \in \mathcal{B}(\mathcal{H})$, $S^{-1} \in \mathcal{B}(\mathcal{H})$, $0 \leq B \in \mathcal{B}_1(\mathcal{H})$ and introduce*

$$T(z) = S + zB, \quad z \in \overline{\mathbb{C}_+}. \tag{4.20}$$

Define $\mathcal{Z} = \mathbb{C}_+ \cup \{x \in \mathbb{R} \,|\, (S + \tau x B)^{-1} \in \mathcal{B}(\mathcal{H})$ for all $\tau \in [0,1]\}$. Then

$$(\log(T(z)) - \log(S)) \in \mathcal{B}_1(\mathcal{H}), \quad z \in \mathcal{Z} \tag{4.21}$$

and

$$\operatorname{tr}(\log(T(z)) - \log(S)) = \sum_{k=1}^{\infty} m_k \int_0^1 d\tau \, \frac{z\lambda_k}{1+\tau z\lambda_k}, \quad z \in \mathcal{Z}, \tag{4.22}$$

where $\{\lambda_k\}_{k\in\mathbb{N}} \subset \mathbb{R}$ is the set of eigenvalues with associated multiplicities $\{m_k\}_{k\in\mathbb{N}}$ of the self-adjoint trace class operator $B^{1/2}S^{-1}B^{1/2}$.

Proof. First one notes that $T(z)$, $z \in \mathcal{Z}$ is invertible. For $z \in \mathbb{R}$ this holds by hypothesis and for $\operatorname{Im}(z) > 0$ this holds since $S^{-1} \in \mathcal{B}(\mathcal{H})$. Thus, $\log(T(z))$ and $\log(S)$ are well-defined. In the following let $z \in \mathcal{Z}$. Since $B \in \mathcal{B}_1(\mathcal{H})$, the representation

$$\log(T(z)) - \log(S) = -i \int_0^{\infty} dt \, ((S + zB + it)^{-1} - (S+it)^{-1}), \tag{4.23}$$

and estimates for the resolvents $(S + iB + it)^{-1}$ and $(S+it)^{-1}$, $t \geq 0$, analogous to those in the proof of Lemma 2.6 of [19] yield (4.21). Therefore,

$$\operatorname{tr}(\log(T(z)) - \log(S)) = -i \operatorname{tr}\bigg(\int_0^{\infty} dt \, ((S+zB+it)^{-1} - (S+it)^{-1})\bigg). \tag{4.24}$$

Based on the estimates in the proof of Lemma 2.6 in [19] mentioned above and the fact that $T = \int_0^\infty ds \, T(s) \in \mathcal{B}_1(\mathcal{H})$ and

$$\operatorname{tr}(T) = \int_0^{\infty} ds \, \operatorname{tr}(T(s)), \tag{4.25}$$

whenever $T(s)$ is continuous with respect to $s \in [0,\infty)$ in $\mathcal{B}_1(\mathcal{H})$-topology and $\|T(s)\|_{\mathcal{B}_1(\mathcal{H})} \leq C(1+s)^{-1-\varepsilon}$ for some $\varepsilon > 0$, one can interchange the integral and the trace in (4.24) and obtain

$$\operatorname{tr}(\log(T(z)) - \log(S)) = -i \int_0^{\infty} dt \, \operatorname{tr}((S+zB+it)^{-1} - (S+it)^{-1})). \tag{4.26}$$

Next, using the fact that $((S + \tau zB + it)^{-1} - (S+it)^{-1})$ is differentiable with respect to τ in trace norm for $(\tau,t) \in [0,1] \times [0,\infty)$ and

$$\begin{aligned}
&(d/d\tau)((S+\tau zB+it)^{-1} - (S+it)^{-1}) \\
&\quad = -(S+\tau zB+it)^{-1} zB (S+\tau zB+it)^{-1}
\end{aligned} \tag{4.27}$$

in trace norm, one concludes

$$\begin{aligned}
&(d/d\tau) \operatorname{tr}((S+\tau zB+it)^{-1} - (S+it)^{-1}) \\
&\quad = -\operatorname{tr}((S+\tau zB+it)^{-1} zB (S+\tau zB+it)^{-1})
\end{aligned}$$

$$= -\operatorname{tr}((S+\tau zB+it)^{-2}zB) \tag{4.28}$$

and hence

$$\operatorname{tr}((S+zB+it)^{-1}-(S+it)^{-1}) = -\int_0^1 d\tau\, \operatorname{tr}(S+\tau zB+it)^{-2}zB), \quad t\geq 0, \tag{4.29}$$

integrating (4.28) from 0 to 1 with respect to τ. Combining (4.26) and (4.29) one obtains

$$\operatorname{tr}(\log(T(z))-\log(S)) = i\int_0^\infty dt \int_0^1 d\tau\ \operatorname{tr}((S+\tau zB+it)^{-2}zB). \tag{4.30}$$

Using the estimate

$$|\operatorname{tr}((S+\tau zB+it)^{-2}B)| \leq \|(S+\tau zB+it)^{-1}\|^2\|B\|_{\mathcal{B}_1(\mathcal{H})} \leq C(1+t^2)^{-1}, \tag{4.31}$$

which holds uniformly with respect to $\tau\in[0,1]$, Fubini's theorem implies

$$\operatorname{tr}(\log(T(z))-\log(S)) = i\int_0^1 d\tau \int_0^\infty dt\ \operatorname{tr}((S+\tau zB+it)^{-2}zB). \tag{4.32}$$

Applying (4.25) again, (4.31) implies

$$\int_0^\infty dt\, \operatorname{tr}((S+\tau zB+it)^{-2}zB) = \operatorname{tr}\bigg(\int_0^\infty dt\,(S+\tau zB+it)^{-2}zB\bigg). \tag{4.33}$$

Using

$$\int_0^\infty dt\,(S+\tau zB+it)^{-2} = -i(S+\tau zB)^{-1}, \tag{4.34}$$

and combining (4.32)–(4.34) one finally gets

$$\begin{aligned}\operatorname{tr}(\log(T(z))-\log(S)) &= \int_0^1 d\tau\ \operatorname{tr}((S+\tau zB)^{-1}zB)\\ &= \int_0^1 d\tau\ \operatorname{tr}(zB^{1/2}(S+\tau zB)^{-1}B^{1/2}).\end{aligned} \tag{4.35}$$

The trace of $zB^{1/2}(S+\tau zB)^{-1}B^{1/2}$, $\tau\in[0,1]$, can easily be computed in terms of the eigenvalues $\{\lambda_k\}_{k\in\mathbb{N}}$ of $B^{1/2}S^{-1}B^{1/2}$. By Lemma 4.1, $zB^{1/2}(S+\tau zB)^{-1}B$ has the eigenvalues

$$\mu_k(\tau,z) = \frac{z\lambda_k}{1+\tau z\lambda_k}, \quad k\in\mathbb{N}, \tag{4.36}$$

with associated multiplicities $\{m_k\}_{k\in\mathbb{N}}$. By Lidskii's theorem (cf. [47, Ch. 3])

$$\operatorname{tr}(zB^{1/2}(S+\tau zB)^{-1}B^{1/2}) = \sum_{k=1}^\infty m_k\mu_k(\tau,z). \tag{4.37}$$

By (4.35) and (4.36)

$$\operatorname{tr}(\log(T(z))-\log(S)) = \int_0^1 d\tau \sum_{k=1}^\infty m_k\mu_k(\tau,z). \tag{4.38}$$

Since $B^{1/2}S^{-1}B^{1/2}\in\mathcal{B}_1(\mathcal{H})$ is self-adjoint, one concludes that $\{\lambda_k\}_{k\in\mathbb{N}}\subset\mathbb{R}$ and that the series $\sum_{k=1}^\infty|\lambda_k|$ converges. Hence, applying the dominated convergence theorem, one can interchange the sum and the integral in (4.38), arriving at (4.22). $\square$

Corollary 4.4. *Under the assumptions of Theorem* 4.3*,*

$$\operatorname{tr}(\operatorname{Im}(\log(S+iB)-\operatorname{Im}(\log(S))) = \operatorname{tr}(\arctan(B^{1/2}S^{-1}B^{1/2})). \tag{4.39}$$

Proof. Pick $z = i$ in Theorem 4.3. Taking the imaginary part of both sides of (4.22), an explicit computation of the integrals in (4.22) yields

$$\operatorname{Im}(\operatorname{tr}(\log(S+iB)) - \operatorname{tr}(\log(S))) = \sum_{k=1}^{\infty} m_k \arctan(\lambda_k) = \operatorname{tr}(\arctan(B^{1/2}S^{-1}B^{1/2})). \tag{4.40}$$

□

Remark 4.5. Corollary 4.4 is an operator analog of the following elementary fact

$$\operatorname{Im}(\log(a+ib)) - \operatorname{Im}(\log(a)) = \arctan(b^{1/2}a^{-1}b^{1/2}), \quad a \in \mathbb{R}\backslash\{0\},\ b>0, \tag{4.41}$$

where $\log(\cdot)$ and $\arctan(\cdot)$ denote the corresponding principal branches, that is,

$$\operatorname{Im}(\log(\lambda)) = 0, \quad \lambda > 0 \text{ and } -\frac{\pi}{2} < \arctan(\lambda) < \frac{\pi}{2},\ \lambda \in \mathbb{R}. \tag{4.42}$$

Theorem 4.3 for $z = 1$, has important consequences when computing the trace of $(\Xi(S+B) - \Xi(S))$ (the case of self-adjoint perturbations).

We start with the simplest case of self-adjoint perturbations where $(S+tB)^{-1} \in \mathcal{B}(\mathcal{H})$ for all $t \in [0,1]$.

Lemma 4.6. *Let $S = S^* \in \mathcal{B}(\mathcal{H})$, $0 \le B \in \mathcal{B}_1(\mathcal{H})$. Assume*

$$(S+tB)^{-1} \in \mathcal{B}(\mathcal{H}) \text{ for all } t \in [0,1]. \tag{4.43}$$

Then

$$\operatorname{tr}(\Xi(S+B) - \Xi(S)) = 0. \tag{4.44}$$

Proof. Under hypothesis (4.43) one can apply Theorem 4.3 for $z = 1$. Thus, $\operatorname{tr}(\Xi(S+B) - \Xi(S)) \in \mathbb{R}$ and therefore (4.44) holds due to (3.4) and the fact that the left-hand side of (4.22) is real. □

Next we relax the condition (4.43) of invertibility of $S + tB$ for all $t \in [0,1]$, still assuming, however, that $S + \tau_0 B$ has a bounded inverse for some $\tau_0 \in \mathbb{R}$. The following result is concerned with the situation where the map $t \mapsto (S+tB)^{-1}$, $t \in [-1,1]$ is singular at some points.

Theorem 4.7. *Let $S = S^* \in \mathcal{B}(\mathcal{H})$, $0 \le B \in \mathcal{B}_1(\mathcal{H})$ and assume $(S+\tau_0 B)^{-1} \in \mathcal{B}(\mathcal{H})$ for some $\tau_0 \in \mathbb{R}$. Then*

$$\operatorname{tr}(\Xi(S+B) - \Xi(S)) = -\sum_{s\in(0,1]} \dim(\ker(S+sB)), \tag{4.45}$$

$$\operatorname{tr}(\Xi(S-B) - \Xi(S)) = \sum_{s\in(-1,0]} \dim(\ker(S+sB)). \tag{4.46}$$

Proof. Since by hypothesis, $(S+\tau_0 B)^{-1} \in \mathcal{B}(\mathcal{H})$, Remark 3.4 implies that $(S+tB)^{-1} \in \mathcal{B}(\mathcal{H})$ for all $t \in [0,1]$ except possibly at a finite number of points $0 = t_0 < t_1 < t_2 < \dots < t_n < t_{n+1} = 1$.

Introducing the notation

$$E(t) = \Xi(S+tB), \quad t \in [0,1] \tag{4.47}$$

one obtains for $\delta > 0$ sufficiently small,

$$\begin{aligned}
&E_{S+B}((-\infty,0)) - E_S((-\infty,0)) = E(1) - E(0) \\
&= \sum_{k=1}^{n+1}(E(t_k) - E(t_k-\delta)) + \sum_{k=1}^{n+1}(E(t_k-\delta) - E(t_{k-1}+\delta)) \\
&+ \sum_{k=1}^{n+1}(E(t_{k-1}+\delta) - E(t_{k-1})). \qquad (4.48)
\end{aligned}$$

By Lemma 4.6,

$$\operatorname{tr}\bigg(\sum_{k=1}^{n+1}(E(t_k-\delta) - E(t_{k-1}+\delta))\bigg) = 0, \qquad (4.49)$$

and by Corollary 3.7 (for $\delta > 0$ sufficiently small),

$$\operatorname{tr}\bigg(\sum_{k=1}^{n+1}(E(t_{k-1}+\delta) - E(t_{k-1}))\bigg) = 0, \qquad (4.50)$$

while

$$\begin{aligned}
&\operatorname{tr}\bigg(\sum_{k=1}^{n+1}(E(t_k) - E(t_k-\delta))\bigg) = -\sum_{k=1}^{n+1}\dim(\ker(S+t_kB)) \\
&= -\sum_{s\in(0,1]}\dim(\ker(S+sB)). \qquad (4.51)
\end{aligned}$$

Combining (4.48)–(4.51) proves (4.45).

Setting $W = S - B$ one gets by (4.45),

$$\begin{aligned}
&\operatorname{tr}\big(\Xi(S) - \Xi(S-B)\big) = \operatorname{tr}\big(\Xi(W+B) - \Xi(W)\big) \\
&= -\sum_{s\in(0,1]}\dim(\ker(W+sB)) = -\sum_{s\in(0,1]}\dim(\ker(S+(s-1)B)) \\
&= -\sum_{s\in(-1,0]}\dim(\ker(S+sB)), \qquad (4.52)
\end{aligned}$$

proving (4.46). ☐

As an immediate consequence one has the following result.

Corollary 4.8. *Assume the hypotheses of Theorem* 4.7. *Then*

$$\begin{aligned}
&\operatorname{tr}(\Xi(S+tB) - \Xi(S)) \\
&= \operatorname{index}(\Xi(S+tB),\Xi(S)) = \begin{cases} -\sum_{s\in(0,t]}\dim(\ker(S+sB)), & t>0, \\ 0, & t=0, \\ \sum_{s\in(t,0]}\dim(\ker(S+sB)), & t<0. \end{cases} \qquad (4.53)
\end{aligned}$$

Remark 4.9. The trace formula (4.53) can be interpreted as follows. The Fredholm index of the pair of spectral projections $(\Xi(S), \Xi(S+B))$ coincides with the number of eigenvalues of $S + sB$ which cross the point 0 from the left to the right as the coupling constant s increases from 0 to 1.

Now, we are prepared to prove our principal result.

Theorem 4.10. *Assume Hypothesis* 3.3. *Then the pair* $(\Xi(S+A+iB),\Xi(S))$ *has a trindex and*

$$\operatorname{trindex}(\Xi(S+A+iB),\Xi(S)) = \frac{1}{\pi}\int_{\mathbb{R}} \frac{dt\, n(t)}{1+t^2}, \tag{4.54}$$

where

$$n(t) = \operatorname{index}(\Xi(S+A+tB),\Xi(S)). \tag{4.55}$$

Proof. By Hypothesis 3.3, $(S+A+tB)^{-1} \in \mathcal{B}(\mathcal{H})$ for all $t>0$ sufficiently small. By Corollary 4.4,

$$\begin{aligned} &\operatorname{tr}(\Xi(S+A+tB+iB) - \Xi(S+A+tB)) \\ &\quad = (1/\pi)\operatorname{tr}(\arctan(B^{1/2}(S+A+tB)^{-1}B^{1/2})). \end{aligned} \tag{4.56}$$

By Lemma 3.5 one concludes that

$$\lim_{t\downarrow 0} \|\Xi(S+A+tB) - \Xi(S+A)\|_{\mathcal{B}_1(\mathcal{H})} = 0 \tag{4.57}$$

and from standard properties of the operator logarithm (cf. [19]) one also infers

$$\lim_{t\downarrow 0} \|\Xi(S+A+iB+tB) - \Xi(S+A+iB)\|_{\mathcal{B}_1(\mathcal{H})} = 0. \tag{4.58}$$

Combining (4.56)–(4.58) one obtains

$$\operatorname{tr}(\Xi(S+A+iB) - \Xi(S+A)) = (1/\pi)\lim_{t\downarrow 0}\operatorname{tr}(\arctan(B^{1/2}(S+A+tB)B^{1/2})) \tag{4.59}$$

and by Theorem 4.2 one infers

$$\operatorname{tr}(\Xi(S+A+iB) - \Xi(S+A)) = \frac{1}{\pi}\int_{\mathbb{R}} \frac{dt\, n^*(t)}{1+t^2} = \frac{1}{\pi}\int_{\mathbb{R}} \frac{dt\, n^*(-t)}{1+t^2}, \tag{4.60}$$

where

$$n^*(-t) = \begin{cases} \sum_{s\in[0,t)} \dim(\ker(sB-S-A)), & t>0, \\ 0, & t=0, \\ -\sum_{s\in[t,0)} \dim(\ker(sB-S-A)), & t<0. \end{cases} \tag{4.61}$$

By Corollary 4.8,

$$n^*(t) = \operatorname{index}(\Xi(S+A+tB),(\Xi(S+A)) \tag{4.62}$$

and therefore,

$$\operatorname{tr}(\Xi(S+A+iB) - \Xi(S+A)) = \frac{1}{\pi}\int_{\mathbb{R}} dt\, \frac{\operatorname{index}(\Xi(S+A+tB),\Xi(S+A))}{1+t^2}. \tag{4.63}$$

Since by (3.30), $(\Xi(S+A)-\Xi(A)) \in \mathcal{B}_\infty(\mathcal{H})$, one concludes that $(\Xi(S+A),\Xi(A))$ is a Fredholm pair of orthogonal projections. Moreover, $(\Xi(S+A+iB)-\Xi(S)) \in \mathcal{B}_1(\mathcal{H})$ implies that the pair $(\Xi(S+A+iB),\Xi(S))$ has a trindex and hence

$$\begin{aligned} &\operatorname{trindex}(\Xi(S+A+iB),\Xi(S)) \\ &\quad = \operatorname{tr}(\Xi(S+A+iB) - \Xi(S+A)) + \operatorname{index}(\Xi(S+A),\Xi(S)). \end{aligned} \tag{4.64}$$

Now (4.54) follows from the chain rule (2.8) for the index of a pair of projections,

$$\begin{aligned} &\operatorname{index}(\Xi(S+A+tB),\Xi(S+A)) + \operatorname{index}(\Xi(S+A),\Xi(S)) \\ &\quad = \operatorname{index}(\Xi(S+A+tB),\Xi(S)), \end{aligned} \tag{4.65}$$

and from the fact that the measure $(1/\pi)(1+t^2)^{-1}dt$ is a probability measure on $\mathbb{R}$. $\square$

Remark 4.11. (i) If $B = 0$, $n(t)$ is independent of t and (4.54) together with $(1/\pi)\int_{\mathbb{R}} dt\,(1+t)^{-2} = 1$ then imply

$$\operatorname{trindex}(\Xi(S+A), \Xi(S)) = \operatorname{index}(\Xi(S+A), \Xi(S)), \tag{4.66}$$

consistent with (2.22).
(ii) The integral (4.54) carries out a "smoothing" of the integer-valued function $n(t)$ resulting in the expression of the trindex of a pair of Ξ-operators.
(iii) Theorem 4.10 shows, in particular, that under Hypothesis 3.3 the difference

$$(\Xi(S+A+iB) - \Xi(S)) \in \mathcal{B}_1(\mathcal{H}) \tag{4.67}$$

if and only if

$$(E_{S+A}((-\infty,0)) - E_S((-\infty,0))) \in \mathcal{B}_1(\mathcal{H}). \tag{4.68}$$

Under hypothesis (4.68) one then obtains

$$\operatorname{trindex}(\Xi(S+A+iB), \Xi(S)) = \operatorname{tr}(\Xi(S+A+iB) - \Xi(S)). \tag{4.69}$$

Remark 4.12. Theorem 4.10 is an operator analog of the fact

$$\operatorname{Im}(\log(a+ib)) - \operatorname{Im}(\log(a)) = \int_{\mathbb{R}} dt(1+t^2)^{-1}(\chi_{(-\infty,0)}(a+tb) - \chi_{(-\infty,0)}(a)), \quad a \in \mathbb{R}\backslash\{0\},\ b>0, \tag{4.70}$$

where $\chi_\Omega(\cdot)$ denotes the characteristic function of $\Omega \subset \mathbb{R}$.

There are two important special cases when (4.68) holds. For instance, if $S = I_{\mathcal{H}}$ or $S = -I_{\mathcal{H}}$ and $A = A^* \in \mathcal{B}_\infty(\mathcal{H})$, the difference (4.68) is even a finite-rank operator,

$$\begin{aligned} \Xi(S+A) - \Xi(S) &= E_{S+A}((-\infty,0)) - E_S((-\infty,0)) \\ &= \begin{cases} E_A((-\infty,-1)), & S = I_{\mathcal{H}}, \\ -E_A([1,\infty)), & S = -I_{\mathcal{H}}. \end{cases} \end{aligned} \tag{4.71}$$

Lemma 4.13. *Assume Hypothesis* 3.3 *and* $S = I_{\mathcal{H}}$ *or* $S = -I_{\mathcal{H}}$. *Then for* $S = I_{\mathcal{H}}$

$$\Xi(I_{\mathcal{H}} + A + iB) \in \mathcal{B}_1(\mathcal{H}) \tag{4.72}$$

and

$$\operatorname{tr}(\Xi(I_{\mathcal{H}} + A + iB)) = \frac{1}{\pi}\int_{\mathbb{R}} \frac{dt\, n_-(t)}{1+t^2}, \tag{4.73}$$

where

$$n_-(t) = \operatorname{rank}(E_{A+tB}((-\infty,-1))) \tag{4.74}$$

is a decreasing right-continuous function. For $S = -I_{\mathcal{H}}$ *one has*

$$(\Xi(-I_{\mathcal{H}} + A + iB) - I_{\mathcal{H}}) \in \mathcal{B}_1(\mathcal{H}) \tag{4.75}$$

and

$$\operatorname{tr}(\Xi(-I_{\mathcal{H}} + A + iB) - I_{\mathcal{H}}) = -\frac{1}{\pi}\int_{\mathbb{R}} \frac{dt\, n_+(t)}{1+t^2}, \tag{4.76}$$

where

$$n_+(t) = \operatorname{rank}(E_{A+tB}([1,\infty))) \tag{4.77}$$

is an increasing right-continuous function.

Proof. Let $S = I_{\mathcal{H}}$. Then $\Xi(S) = \Xi(I_{\mathcal{H}}) = 0$ and

$$\operatorname{index}(\Xi(I_{\mathcal{H}} + A + tB), \Xi(I_{\mathcal{H}})) = \operatorname{tr}(\Xi(I_{\mathcal{H}} + A + tB)) = \operatorname{rank}(E_{A+tB}((-\infty, -1))), \tag{4.78}$$

prove (4.73) and (4.74). Next, let $S = -I_{\mathcal{H}}$. Then $\Xi(S) = \Xi(-I_{\mathcal{H}}) = I_{\mathcal{H}}$ and

$$\begin{aligned}&\operatorname{index}(\Xi(-I_{\mathcal{H}} + A + tB), \Xi(-I_{\mathcal{H}})) = \operatorname{tr}((\Xi(-I_{\mathcal{H}} + A + tB) - I_{\mathcal{H}}) \\ &\quad = -\operatorname{tr}(E_{-I_{\mathcal{H}}+A+tB}([0, \infty))) = -\operatorname{rank}(E_{A+tB}([1, \infty)))\end{aligned} \tag{4.79}$$

prove (4.76) and (4.77). □

Theorem 4.10 admits the following immediate extension.

Corollary 4.14. *Assume that the triples (S, A_1, B_1) and (S, A_2, B_2) satisfy Hypothesis 3.3. Then the pair $(\Xi(S + A_1 + iB_1), \Xi(S + A_2 + iB_2))$ has a generalized trace and*

$$\operatorname{gtr}(\Xi(S + A_1 + iB_1), \Xi((S + A_2 + iB_2)) = \frac{1}{\pi}\int_{\mathbb{R}} \frac{dt\, n(t)}{1+t^2}, \tag{4.80}$$

where

$$n(t) = \operatorname{index}(\Xi(S + A_1 + tB_1), \Xi((S + A_2 + tB_2)). \tag{4.81}$$

Proof. By Theorem 4.10 the pairs $(\Xi(S + A_1 + iB_1), \Xi(S))$ and $(\Xi(S + A_2 + iB_2), \Xi(S))$ have a trindex and hence the pair $(\Xi(S + A_1 + iB_1), \Xi(S + A_2 + iB_2))$ has a generalized trace and

$$\begin{aligned}&\operatorname{gtr}(\Xi(S + A_1 + iB_1), \Xi(S + A_2 + iB_2)) \\ &\quad = \operatorname{trindex}(\Xi(S + A_1 + B_1), \Xi(S)) - \operatorname{trindex}(\Xi(S + A_2 + iB_2), \Xi(S)).\end{aligned} \tag{4.82}$$

Moreover, the following representations hold

$$\operatorname{trindex}(\Xi(S + A_1 + iB_1), \Xi(S)) = \frac{1}{\pi}\int_{\mathbb{R}} \frac{dt \operatorname{index}(\Xi(S + A_1 + tB_1), \Xi(S))}{1+t^2}, \tag{4.83}$$

$$\operatorname{trindex}(\Xi(S + A_2 + iB_2), \Xi(S)) = \frac{1}{\pi}\int_{\mathbb{R}} \frac{dt \operatorname{index}(\Xi(S + A_2 + tB_2), \Xi(S))}{1+t^2}. \tag{4.84}$$

Under Hypothesis 3.3, $(\Xi(S + A_j + tB_j) - \Xi(S)) \in \mathcal{B}_\infty(\mathcal{H})$, $j = 1, 2$ and hence, by Theorem 2.2 (i),

$$\begin{aligned}&\operatorname{index}(\Xi(S + A_1 + tB_1), \Xi(S)) - \operatorname{index}(\Xi(S + A_2 + tB_2), \Xi(S)) \\ &\quad = \operatorname{index}(\Xi(S + A_1 + tB_1), \Xi(S + A_2 + iB_2)).\end{aligned} \tag{4.85}$$

Combining (4.82)–(4.85) proves (4.80) and (4.81). □

Finally, we turn to a version of the Birman-Krein formula [7].

Theorem 4.15. *Under Hypothesis 3.3, the operator*

$$\mathbf{S} = I_{\mathcal{H}} - 2iB^{1/2}(S + A + iB)^{-1}B^{1/2} \tag{4.86}$$

is unitary, $(\mathbf{S} - I_{\mathcal{H}}) \in \mathcal{B}_1(\mathcal{H})$ and its Fredholm determinant can be represented as follows

$$\det(\mathbf{S}) = \exp(-2\pi i \operatorname{trindex}(\Xi(S + A + iB), \Xi(S))). \tag{4.87}$$

Proof. Introduce the family of trace class operators

$$\mathcal{A}(z) = B^{1/2}(S + A + zB)^{-1}B^{1/2}, \quad \operatorname{Im}(z) > 0. \tag{4.88}$$

Then,

$$\mathbf{S} = I_{\mathcal{H}} - 2i\mathcal{A}(i), \quad (\mathbf{S} - I_{\mathcal{H}}) \in \mathcal{B}_1(\mathcal{H}) \tag{4.89}$$

and hence the Fredholm determinant of $\mathbf{S}$ is well-defined. By the analytic Fredholm theorem the set of $z \in \mathbb{C}$ such that $S + A + zB$ does not have a bounded inverse is discrete and therefore there exists a $\delta > 0$ such that $\mathcal{A}(\delta)$ is well-defined. By Lemma 4.1, the operator $\mathcal{A}(\delta)$ has the eigenvalue δ^{-1} if and only if $\dim(\ker(S + A)) \neq 0$ with associated multiplicity equal to $\dim(\ker(S + A))$.

Let $\{\mu_k(\delta)\}_{k\in\mathbb{N}} = \operatorname{spec}(\mathcal{A}(\delta))\backslash\{\delta^{-1}\}$ different from the eigenvalue δ^{-1} with multiplicities $\{m_k\}_{k\in\mathbb{N}}$. By Lemma 4.1, $\mathcal{A}(i)$ has the eigenvalues

$$\mu_k(i) = \frac{\mu_k(\delta)}{1 - \mu_k(\delta)(\delta - i)}, \quad k \in \mathbb{N}, \tag{4.90}$$

with multiplicities $\{m_k\}_{k\in\mathbb{N}}$ and, in addition, the eigenvalue $-i$ of multiplicity $\dim(\ker(S + A))$ (if $(S + A)$ has a nontrivial kernel). Moreover, $\mathcal{A}(i)$ has no other eigenvalues different from zero. Therefore, by (4.89),

$$\det(\mathbf{S}) = (-1)^{\dim(\ker(S+A))} \prod_{k=1}^{\infty} \left(\frac{1 - \mu_k(\delta)\delta - i\mu_k(\delta)}{1 - \mu_k(\delta)\delta + i\mu_k(\delta)}\right)^{m_k}. \tag{4.91}$$

Moreover,

$$\begin{aligned}
&\operatorname{trindex}(\Xi(S + A + iB), \Xi(S)) \\
&= \operatorname{tr}(\Xi(S + A + iB) - \Xi(S + A)) + \operatorname{index}(\Xi(S + A), \Xi(S)) \\
&= (1/\pi) \lim_{\varepsilon\downarrow 0} \operatorname{tr}(\arctan(B^{1/2}(S + A + \varepsilon B)^{-1}B^{1/2})) + \operatorname{index}(\Xi(S + A), \Xi(S)) \\
&= (1/\pi) \sum_{k=1}^{\infty} m_k \arctan(\mu_k(\delta)(1 - \mu_k(\delta)\delta)^{-1}) + (1/2)\dim(\ker(S + A)) + n,
\end{aligned} \tag{4.92}$$

for some $n \in \mathbb{Z}$. Combining (4.91) and (4.92) results in (4.87). $\square$

To avoid additional technicalities we only treated the case where S is bounded. It is clear that our formalism in Section 3 extends to unbounded dissipative operators T in $\mathcal{H}$, but such an extension will be discussed elsewhere.

5. Some Applications

The main purpose of this section is to obtain new representations for Krein's spectral shift function associated with a pair of self-adjoint operators (H_0, H) and to provide a generalization of the classical Birman-Schwinger principle, replacing the traditional eigenvalue counting functions by appropriate spectral shift functions.

We start with our representation of Krein's spectral shift function and temporarily assume the following hypothesis.

Hypothesis 5.1. *Let H_0 be a self-adjoint operator in $\mathcal{H}$ with domain* $\operatorname{dom}(H_0)$*, J a bounded self-adjoint operator with $J^2 = I_{\mathcal{H}}$, and $K \in \mathcal{B}_2(\mathcal{H})$ a Hilbert-Schmidt operator.*

Introducing

$$V = KJK^* \tag{5.1}$$

we define the self-adjoint operator H in $\mathcal{H}$ by

$$H = H_0 + V, \quad \mathrm{dom}(H) = \mathrm{dom}(H_0). \tag{5.2}$$

We could have easily incorporated the case where K maps between different Hilbert spaces but we omit the corresponding details. Moreover, we introduce the following bounded operator in $\mathcal{H}$,

$$\Phi(z) = J + K^*(H_0 - z)^{-1}K : \mathcal{H} \to \mathcal{H}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{5.3}$$

One easily verifies (cf. [19, Sect. 3]) that $\Phi(z)$ is an operator-valued Herglotz function in $\mathcal{H}$ (i.e., $\mathrm{Im}(\Phi(z)) \geq 0$ for all $z \in \mathbb{C}_+$) and that

$$\Phi(z)^{-1} = J - JK^*(H - z)^{-1}KJ, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{5.4}$$

In the following it is convenient to choose

$$J = \mathrm{sgn}(V), \tag{5.5}$$

where in the present context the sign function is defined by $\mathrm{sgn}(x) = 1$ if $x \geq 0$ and $\mathrm{sgn}(x) = -1$ if $x < 0$. Next, let $\{P_n\}_{n\in\mathbb{N}}$ be a family of finite-rank spectral projections of V satisfying,

$$\operatorname*{s-lim}_{n\to\infty} P_n = I_{\mathcal{H}}. \tag{5.6}$$

Introducing the finite-rank operators

$$K_n = KP_n, \quad V_n = (K_n)J(K_n)^*, \quad n \in \mathbb{N}, \tag{5.7}$$

one infers (cf. e.g., [23])

$$\lim_{n\to\infty} \|V_n - V\|_{\mathcal{B}_1(\mathcal{H})}. \tag{5.8}$$

Together with the operator-valued Herglotz function $\Phi(z)$ given by (5.3), we introduce the family of operator-valued Herglotz functions

$$\Phi_n(z) = J + K_n^*(H_0 - z)^{-1}K_n : \mathcal{H} \to \mathcal{H}, \tag{5.9}$$

and its finite-rank restriction

$$\Psi_n(z) = P_n\Phi_n(z)P_n : P_n\mathcal{H} \to P_n\mathcal{H}. \tag{5.10}$$

One computes as in (5.4),

$$\Phi_n^{-1}(z) = J - JK_n^*(H_n - z)^{-1}K_nJ, \tag{5.11}$$

where

$$H_n = H_0 + V_n, \quad \mathrm{dom}(H_n) = \mathrm{dom}(H_0). \tag{5.12}$$

Consequently,

$$\Psi_n^{-1}(z) = \Phi_n^{-1}(z)|_{P_n\mathcal{H}} \text{ in } P_n\mathcal{H}. \tag{5.13}$$

Since $\Psi_n(z)$, $z \in \mathbb{C}_+$ is invertible in $P_n\mathcal{H}$, one infers from [21] (see also, [13]) the existence of a family of operators $\{\Xi_n(\lambda)\}$ defined for (Lebesgue) a.e. $\lambda \in \mathbb{R}$, satisfying

$$0 \leq \Xi_n(\lambda) \leq I_n \text{ for a.e. } \lambda \in \mathbb{R}, \tag{5.14}$$

where I_n denotes the identity operator in $P_n\mathcal{H}$, and

$$\log(\Psi_n(z)) = C_n + \int_{\mathbb{R}} d\lambda\, \Xi_n(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{5.15}$$

$$C_n = C_n^* = \mathrm{Re}(\log \Psi_n(i)), \tag{5.16}$$

$$\Xi_n(\lambda) = \pi^{-1} \lim_{\varepsilon\downarrow 0} \mathrm{Im}(\log(\Psi_n(\lambda + i\varepsilon)) \text{ for a.e. } \lambda \in \mathbb{R}. \tag{5.17}$$

Next, we briefly recall the notion of Krein's spectral shift function for a pair of self-adjoint operators in $\mathcal{H}$ (cf. e.g., [4, Sect. 19.1], [7], [8], [11], [12], [27], [29], [31], [32], [33], [34], [40], [42], [50], [53, Ch. 8] and the literature cited therein), a concept originally introduced by Lifshitz [35], [36]. Assuming $\mathrm{dom}(H_0) = \mathrm{dom}(H)$ and $(H - H_0) \in \mathcal{B}_1(\mathcal{H})$ (this could be considerably relaxed but suffices for our present purpose), Krein's (real-valued) spectral shift function $\xi(\lambda, H_0, H)$ is uniquely defined for a.e. $\lambda \in \mathbb{R}$ by

$$\xi(\cdot, H_0, H) \in L^1(\mathbb{R}; d\lambda),$$

$$\mathrm{tr}((H - z)^{-1} - (H_0 - z)^{-1}) = -\int_{\mathbb{R}} d\lambda\, \xi(\lambda, H_0, H)(\lambda - z)^{-2}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{5.18}$$

Lemma 5.2. *Denote by* $\xi(\lambda, H_0, H_n)$ *the spectral shift function associated with the pair* (H_0, H_n)*. Then*

$$\xi(\lambda, H_0, H_n) = \mathrm{tr}_{P_n\mathcal{H}}(\Xi_n(\lambda)) - N_n \text{ for a.e. } \lambda \in \mathbb{R}, \tag{5.19}$$

where

$$N_n = \#\{\text{of strictly negative eigenvalues of } V_n, \text{ counting multiplicity}\}. \tag{5.20}$$

Proof. Differentiating $\mathrm{tr}_{P_n\mathcal{H}}(\log(\Psi_n(z)))$ with respect to z (c.f., [22, Sect. IV.1])

$$(d/dz)\, \mathrm{tr}_{P_n\mathcal{H}}(\log(\Psi_n(z)) = \mathrm{tr}_{P_n\mathcal{H}}(\Psi_n^{-1}(z)\Psi_n'(z)), \tag{5.21}$$

one obtains by (5.9) and (5.13)

$$\mathrm{tr}_{P_n\mathcal{H}}(\Psi_n^{-1}(z)\Psi_n'(z)) = \mathrm{tr}_{\mathcal{H}}(P_n\Phi_n^{-1}(z)P_nP_n\Phi_n'(z)P_n) = \mathrm{tr}_{\mathcal{H}}(\Phi_n^{-1}(z)\Phi_n'(z)), \tag{5.22}$$

since $(d/dz)\Phi_n(z) = (d/dz)P_n\Phi_n(z)P_n$. However, $\mathrm{tr}_{\mathcal{H}}(\Phi_n^{-1}(z)\Phi_n'(z))$ can be computed explicitly,

$$\begin{aligned}
&\mathrm{tr}_{\mathcal{H}}((\Phi_n^{-1}(z)\Phi_n'(z)) \\
&= \mathrm{tr}_{\mathcal{H}}(J - JK_n^*(H_n - z)^{-1}K_nJ)K_n^*(H_0 - z)^{-2}K_n) \\
&= \mathrm{tr}_{\mathcal{H}}(K_n(J - JK_n^*(H_n - z)^{-1}K_nJ)K_n^*(H_0 - z)^{-2}) \\
&= \mathrm{tr}_{\mathcal{H}}(H_0 - z)^{-1}K_n(J - JK_n^*(H_n - z)^{-1}K_nJ)K_n^*(H_0 - z)^{-1}) \\
&= \mathrm{tr}((H_0 - z)^{-1}K_nJK_n^*(H_0 - z)^{-1}) \\
&- \mathrm{tr}_{\mathcal{H}}((H_0 - z)^{-1}K_nJK_n^*(H_n - z)^{-1}K_nJK_n^*(H_0 - z)^{-1}) \\
&= \mathrm{tr}_{\mathcal{H}}((H_0 - z)^{-1}V_n(H_0 - z)^{-1} - (H_0 - z)^{-1}V_n(H_n - z)^{-1}V_n(H_0 - z)^{-1}) \\
&= -\,\mathrm{tr}_{\mathcal{H}}((H_n - z)^{-1} - (H_0 - z)^{-1}) \quad z \in \mathbb{C}\backslash\mathbb{R},
\end{aligned} \tag{5.23}$$

iterating the second resolvent identity. Combining (5.21)–(5.23) one infers

$$(d/dz)\, \mathrm{tr}_{P_n\mathcal{H}}(\log(\Psi_n(z)) = -\,\mathrm{tr}_{\mathcal{H}}((H_n - z)^{-1} - (H_0 - z)^{-1}). \tag{5.24}$$

Taking traces in (5.15) one gets

$$\operatorname{tr}_{P_n\mathcal{H}}(\log(\Psi_n(z))) = \operatorname{tr}_{P_n\mathcal{H}}(C_n) + \int_{\mathbb{R}} d\lambda \ \operatorname{tr}_{P_n\mathcal{H}}(\Xi_n(\lambda))((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \tag{5.25}$$

and thus, differentiating (5.25) with respect to z,

$$(d/dz)\operatorname{tr}(\log(\Psi_n(z))) = \int_{\mathbb{R}} d\lambda \ \operatorname{tr}(\Xi_n(\lambda))(\lambda - z)^{-2}. \tag{5.26}$$

Comparing (5.26) and (5.24) one arrives at the trace formula

$$\int_{\mathbb{R}} d\lambda \ \operatorname{tr}(\Xi_n(\lambda))(\lambda - z)^{-2} = -\operatorname{tr}((H_n - z)^{-1} - (H_0 - z)^{-1}), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{5.27}$$

and hence up to an additive constant, $\operatorname{tr}(\Xi_n(\lambda))$ coincides with the spectral shift function $\xi(\lambda, H_0, H_n)$ associated with the pair (H_0, H_n) for a.e. $\lambda \in \mathbb{R}$.

Next we determine this constant. Introducing $J_n = J\big|_{P_n\mathcal{H}}$, $J_n^2 = I_n$, one obtains

$$\begin{aligned}\log(J_n) &= i\operatorname{Im}(\log(J_n)) \\ &= \pi^{-1}\int_{\mathbb{R}} d\lambda \operatorname{Im}(\log(J_n))((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}).\end{aligned} \tag{5.28}$$

Moreover,

$$\pi^{-1}\operatorname{tr}_{P_n\mathcal{H}}(\operatorname{Im}(\log((J_n))) = N_n, \tag{5.29}$$

where N_n denotes the number of strictly negative eigenvalues of J_n, counting multiplicity. Thus, N_n coincides with the number of strictly negative eigenvalues of V_n. Combining (5.28), (5.29), and using (5.15) results in

$$\begin{aligned}&\log(\Psi_n(z)) - \log(J_n) \\ &= C_n + \int_{\mathbb{R}} d\lambda\,(\Xi_n(\lambda) - \pi^{-1}\operatorname{Im}(\log((J_n)))((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1})\end{aligned} \tag{5.30}$$

and hence in

$$\operatorname{tr}_{P_n\mathcal{H}}(\operatorname{Im}(\log(\Psi_n(z)) - \log(J_n))) = \int_{\mathbb{R}} d\lambda\,(\operatorname{tr}(\Xi_n(\lambda)) - N_n)\frac{\operatorname{Im}(z)}{(\lambda - \operatorname{Re}(z))^2 + \operatorname{Im}(z)^2}. \tag{5.31}$$

Since $||(H_0 - iy)^{-1}|| = O(|y|^{-1})$ as $y \uparrow +\infty$, one concludes

$$y||\log(\Psi_n(iy)) - \log(J_n)|| = O(1) \text{ as } y \uparrow +\infty \tag{5.32}$$

and hence that $y\operatorname{Im}(\operatorname{tr}_{P_n\mathcal{H}}(\log(\Psi_n(iy)) - \log(J_n)))$ is bounded as $y \uparrow +\infty$. In particular, (5.31) and (5.32) imply that

$$\xi_n(\lambda) = \operatorname{tr}_{P_n\mathcal{H}}(\Xi_n(\lambda)) - N_n \tag{5.33}$$

is integrable,

$$\xi_n(\cdot) \in L^1(\mathbb{R}; d\lambda). \tag{5.34}$$

Since

$$\int_{\mathbb{R}} d\lambda(\lambda - z)^{-2} = 0 \text{ for all } z \in \mathbb{C},\ \operatorname{Im}(z) \neq 0, \tag{5.35}$$

(5.33) and (5.27) yield the trace formula

$$\int_{\mathbb{R}} d\lambda\,\xi_n(\lambda)(\lambda - z)^{-2} = \int_{\mathbb{R}} d\lambda \ \operatorname{tr}_{P_n\mathcal{H}}(\Xi_n(\lambda))(\lambda - z)^{-2}$$

$$= -\operatorname{tr}_{\mathcal{H}}((H_n - z)^{-1} - (H_0 - z)^{-1}), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{5.36}$$

which together with (5.34) proves (5.19), (5.20). ☐

Theorem 5.3. *Assume Hypothesis* 5.1 *and fix a* $p > 1$. *Moreover, let* $V = KJK^*$, *where* $J = \operatorname{sgn}(V)$. *Then the spectral shift function* $\xi(\lambda, H_0, H)$ *associated with the pair* (H_0, H), $H = H_0 + V$ *admits the representation*

$$\xi(\lambda, H_0, H) = \operatorname{trindex}(\Xi(J + K^*(H_0 - \lambda - i0)^{-1}K), \Xi(J)) \text{ for a.e. } \lambda \in \mathbb{R}, \tag{5.37}$$

where $K^*(H_0 - \lambda - i0)^{-1}K$ *is defined as*

$$\lim_{\varepsilon \downarrow 0} \|K^*(H_0 - \lambda - i0)^{-1}K - K^*(H_0 - \lambda - i\varepsilon)^{-1}K\|_{\mathcal{B}_p(\mathcal{H})} = 0 \text{ for a.e. } \lambda \in \mathbb{R}. \tag{5.38}$$

Proof. First of all, one notes that the boundary values $K^*(H_0 - \lambda - i0)^{-1}K$ and $K^*(H - \lambda - i0)^{-1}K$ exist λ a.e. in the topology $\mathcal{B}_p(\mathcal{H})$ for every $p > 1$ (but in general not for $p = 1$,) [38], [39] (see also [4, Ch. 3], [6], [15]). By (5.4), the operator $J + K^*(H_0 - \lambda - i0)^{-1}K$ has a bounded inverse for a.e. $\lambda \in \mathbb{R}$. Moreover (see, e.g., [4, Sect. I.3.4]),

$$\lim_{\varepsilon \downarrow 0} \|\operatorname{Im}(K^*(H_0 - \lambda - i\varepsilon)^{-1}K) - \operatorname{Im}(K^*(H_0 - \lambda - i0)^{-1}K)\|_{\mathcal{B}_1(\mathcal{H})} = 0 \quad \text{for a.e. } \lambda \in \mathbb{R}. \tag{5.39}$$

Thus, there exists a set $\Lambda \subset \mathbb{R}$ with $|\mathbb{R}\backslash\Lambda| = 0$ ($|\cdot|$ denoting Lebesgue measure on $\mathbb{R}$) satisfying the following properties. For any $\lambda \in \Lambda$:
(i) The boundary values $\Phi(\lambda + i0) = \lim_{\varepsilon\downarrow 0} \Phi(\lambda + i\varepsilon)$ exist in $\mathcal{B}_p(\mathcal{H})$-topology (cf. (5.3)).
(ii) The operator $\Phi(\lambda + i0)$ has a bounded inverse.
(iii) $\operatorname{Im}(\Phi(\lambda + i\varepsilon))$ converges to $\operatorname{Im}(\Phi(\lambda + i0))$ as $\varepsilon \downarrow 0$ in $\mathcal{B}_1(\mathcal{H})$-topology.

For any $n \in \mathbb{N}$, $\lambda \in \Lambda$ introduce the function

$$\xi_n(\lambda) = \operatorname{trindex}(\Xi(P_n\Phi(\lambda + i0)P_n, \Xi(P_nJP_n)). \tag{5.40}$$

Since P_n commute with J and the subspace $P_n\mathcal{H}$ is invariant for $J + P_nK^*(H_0 - \lambda - i0)^{-1}KP_n$ one concludes by (5.40) that (cf. (2.23))

$$\begin{aligned} \xi_n(\lambda) &= \operatorname{tr}(\Xi(J + P_nK^*(H_0 - \lambda - i0)^{-1}KP_n) - \Xi(J)) \\ &= \operatorname{trindex}(\Xi(J + P_nK^*(H_0 - \lambda - i0)^{-1}KP_n), \Xi(J)), \quad \lambda \in \Lambda. \end{aligned} \tag{5.41}$$

On the other hand, by Lemma 5.2, (5.9), and (5.10) one infers that the function $\xi_n(\lambda)$ coincides with the spectral shift function $\xi(\lambda, H_0, H_n)$ associated with the pair (H_0, H_n)

$$\xi_n(\lambda) = \xi(\lambda, H_0, H_n), \text{ a.e. } \lambda \in \mathbb{R}, \tag{5.42}$$

where H_n is given by (5.12). By a result of Grümm [23], properties (i)–(iii), and (5.6), one obtains for $\lambda \in \Lambda$,

$$\lim_{n\to\infty} \|(\operatorname{Re}(P_nK^*(H_0 - \lambda - i0)^{-1}KP_n) - \operatorname{Re}(K^*(H_0 - \lambda - i0)^{-1}K)\|_{\mathcal{B}_p(\mathcal{H})} = 0, \tag{5.43}$$

$$\lim_{n\to\infty} \|(\operatorname{Im}(P_nK^*(H_0 - \lambda - i0)^{-1}KP_n) - \operatorname{Im}(K^*(H_0 - \lambda - i0)^{-1}K)\|_{\mathcal{B}_1(\mathcal{H})} = 0. \tag{5.44}$$

Applying the approximation Theorem 3.12 then yields

$$\lim_{n\to\infty}\xi_n(\lambda)=\operatorname{trindex}(\Xi(\Phi(\lambda+i0),\Xi(J)),\quad \lambda\in\Lambda \text{ pointwise.} \tag{5.45}$$

Convergence (5.8) of V_n to V in trace norm implies the convergence of the corresponding spectral shift functions $\xi_n(\lambda)$ to the spectral shift function $\xi(\lambda,H_0,H)$ in $L^1(\mathbb{R})$. This in turn implies the existence of a subsequence $\{\xi_{n_k}(\lambda)\}_{k\in\mathbb{N}}$ converging pointwise a.e. Together with (5.45) this proves (5.37). □

Remark 5.4. Let $\Lambda=\{\lambda\in\mathbb{R}\,|\,\text{s.t. } A(\lambda) \text{ and } B(\lambda) \text{ exist, } A(\lambda)\in\mathcal{B}_2(\mathcal{H}),B(\lambda)\in\mathcal{B}_1(\mathcal{H}), \text{ and } (J+A(\lambda)+iB(\lambda))^{-1}\in\mathcal{B}(\mathcal{H})\}$. Then, as shown in Corollary 3.10, the condition

$$[A(\lambda),J]\notin\mathcal{B}_1(\mathcal{H}) \tag{5.46}$$

is necessary and sufficient for the validity of

$$(\Xi(J+A(\lambda)+iB(\lambda))-\Xi(J))\notin\mathcal{B}_1(\mathcal{H}). \tag{5.47}$$

Next, note that the following three conditions,

$$(i)\,\operatorname{rank}(E_V((-\infty,0))=\operatorname{rank}(E_V((0,\infty))=\infty, \tag{5.48}$$

$$(ii)\,\lambda\in\operatorname{ess.spec}(H_0), \tag{5.49}$$

$$(iii)\,A(\lambda)\notin\mathcal{B}_1(\mathcal{H}), \tag{5.50}$$

are a consequence of condition (5.46). Thus, if at least one of the conditions (i)–(iii) is violated, the ξ-function (c.f., (5.37)) can be represented in the simple form

$$\xi(\lambda,H_0,H)=\operatorname{tr}(\Xi(J+K^*(H_0-\lambda-i0)^{-1}K)-\Xi(J)), \tag{5.51}$$

and the concept of a trindex becomes redundant in this case. On the other hand, there are of course examples (c.f., Remark 3.11), where

$$|\{\lambda\in\mathbb{R}\,|\,(\Xi(J+|V|^{1/2}(H_0-\lambda-i0)^{-1}|V|^{1/2})-\Xi(J))\notin\mathcal{B}_1(\mathcal{H})\}|>0, \tag{5.52}$$

with $|\cdot|$ denoting Lebesgue measure on $\mathbb{R}$. A concrete example illustrating (5.52) can be constructed as follows. Consider an infinite dimensional complex separable Hilbert space $\mathcal{K}$, an operator $0\le k=k^*\in\mathcal{B}_2(\mathcal{K})\backslash\mathcal{B}_1(\mathcal{K})$, with $\ker(k)=\{0\}$, and a self-adjoint operator h_0 in $\mathcal{K}$ such that

$$a(\lambda)=\operatorname*{n-lim}_{\varepsilon\to0}\operatorname{Re}(k(h_0-\lambda-i\varepsilon)^{-1}k)\notin\mathcal{B}_1(\mathcal{K}) \text{ for a.e. } \lambda\in\mathbb{R}. \tag{5.53}$$

Existence of such $\mathcal{K}$, k, and h_0 can be inferred from [38]. Next, define $\mathcal{H}=\mathcal{K}\oplus\mathcal{K}$ and introduce $H_0=\left(\begin{smallmatrix}h_0&0\\0&0\end{smallmatrix}\right)$, $V=i\left(\begin{smallmatrix}0&k^2\\-k^2&0\end{smallmatrix}\right)$. Then $J=\operatorname{sgn}(V)=i\left(\begin{smallmatrix}0&I_{\mathcal{K}}\\-I_{\mathcal{K}}&0\end{smallmatrix}\right)$, $|V|^{1/2}=\left(\begin{smallmatrix}k&0\\0&k\end{smallmatrix}\right)$, and

$$A(\lambda)=\operatorname*{n-lim}_{\varepsilon\to0}\operatorname{Re}(|V|^{1/2}(H_0-\lambda-i\varepsilon)^{-1}|V|^{1/2})=\begin{pmatrix}a(\lambda)&0\\0&-(1/\lambda)k^2\end{pmatrix} \tag{5.54}$$

for a.e. $\lambda\in\mathbb{R}\backslash\{0\}$. Moreover, one computes

$$[A(\lambda),J]=i\begin{pmatrix}0&a(\lambda)+(1/\lambda)k^2\\a(\lambda)+(1/\lambda)k^2&0\end{pmatrix}\notin\mathcal{B}_1(\mathcal{H}) \text{ for a.e. } \lambda\in\mathbb{R}, \tag{5.55}$$

since $k^2\in\mathcal{B}_1(\mathcal{K})$.

As a consequence of Theorems 4.10 and 5.3 one has the following representation for the spectral shift function via the integral of the index of a Fredholm pair of spectral projections.

Theorem 5.5. *Assume Hypothesis* 5.1 *and introduce* $V = KJK^*$. *In addition, for a.e.* $\lambda \in \mathbb{R}$, *let* $A(\lambda) + iB(\lambda)$ *be the normal boundary values of the operator-valued Herglotz function* $K^*(H_0 - z)^{-1}K$ *on the real axis, that is,*

$$A(\lambda) = \operatorname*{n-lim}_{\varepsilon\downarrow 0} \operatorname{Re}(K^*(H_0 - \lambda - i\varepsilon)^{-1}K) \text{ for a.e. } \lambda \in \mathbb{R} \tag{5.56}$$

and

$$B(\lambda) = \operatorname*{n-lim}_{\varepsilon\downarrow 0} \operatorname{Im}(K^*(H_0 - \lambda - i\varepsilon)^{-1}K) \text{ for a.e. } \lambda \in \mathbb{R}. \tag{5.57}$$

Then

$$\xi(\lambda, H_0, H) = \frac{1}{\pi}\int_{\mathbb{R}} dt \frac{\operatorname{index}\big(E_{J+A(\lambda)+tB(\lambda)}((-\infty,0)), E_J((-\infty,0))\big)}{1+t^2} \quad \text{for a.e. } \lambda \in \mathbb{R}. \tag{5.58}$$

In the particular case of sign-definite perturbations, that is, $J = I_{\mathcal{H}}$ or $J = -I_{\mathcal{H}}$, applying Lemma 4.13 yields the following result originally due to Pushnitski [40], representing the spectral shift function in terms of an integrated eigenvalue counting function.

Corollary 5.6. (Pushnitski [40].) *Let* $0 \le V \in \mathcal{B}_1(\mathcal{H})$ *and* $H_0 = H_0^*$. *Then the spectral shift function* $\xi(\lambda, H_0, H_0 \pm V)$ *associated with the pair* $(H_0, H_0 \pm V)$ *admits the representation*

$$\xi(\lambda, H_0, H_0 \pm V) = \pm\frac{1}{\pi}\int_{\mathbb{R}} dt \frac{\operatorname{rank}(E_{\mp(A(\lambda)+tB(\lambda))}((1,\infty)))}{1+t^2}. \tag{5.59}$$

Remark 5.7. (i) Strictly speaking, a direct application of Lemma 4.13 in the case of nonpositive perturbations would give the representation

$$\xi(\lambda, H_0, H_0 - V) = -\frac{1}{\pi}\int_{\mathbb{R}} dt \frac{\operatorname{rank}(E_{A(\lambda)+tB(\lambda)}([1,\infty)))}{1+t^2}, \tag{5.60}$$

which, however, yields the same result as in (5.59), since

$$\int_{\mathbb{R}} dt \frac{\operatorname{rank}(E_{A(\lambda)+tB(\lambda)}(\{1\}))}{1+t^2} = 0 \text{ for a.e. } \lambda \in \mathbb{R}. \tag{5.61}$$

(ii) In the special case where $\lambda \in \mathbb{R}\backslash\{\operatorname{spec}(H_0) \cup \operatorname{spec}(H)\}$, (5.58) turns into

$$\begin{aligned} \xi(\lambda, H_0, H) &= \operatorname{index}(E_{J+A(\lambda)}((-\infty,0)), E_J((-\infty,0))) \\ &= \operatorname{tr}(E_{J+A(\lambda)}((-\infty,0)) - E_J((-\infty,0))). \end{aligned} \tag{5.62}$$

In the particular cases of sign-definite perturbations ($J = \pm I_{\mathcal{H}}$) one obtains

$$\xi(\lambda, H_0, H_0 \pm V) = \pm\operatorname{rank}(E_{\mp A(\lambda)}((1,\infty))), \tag{5.63}$$

since $\operatorname{rank}(E_{\mp A(\lambda)}(\{1\})) = 0$ for a.e. $\lambda \in \mathbb{R}$. The result (5.63) is due to Sobolev [51].

The trindex representation (5.37) for $\xi(\lambda, H_0, H)$ enables us to introduce a new generalized spectral shift function outside the trace-class perturbation scheme under rather weak assumptions on $H - H_0$. First we recall the following exponential representation for operator-valued Herglotz functions partially proven in [19].

Theorem 5.8. *Suppose $M : \mathbb{C}_+ \to \mathcal{B}(\mathcal{H})$ is an operator-valued Herglotz function and $M(z_0)^{-1} \in \mathcal{B}(\mathcal{H})$ for some (and hence for all) $z_0 \in \mathbb{C}_+$. Then there exists a family of bounded self-adjoint weakly (Lebesgue) measurable operators $\{\widehat{\Xi}(\lambda)\}_{\lambda\in\mathbb{R}} \subset \mathcal{B}(\mathcal{H})$,*

$$0 \leq \widehat{\Xi}(\lambda) \leq I_{\mathcal{H}} \text{ for a.e. } \lambda \in \mathbb{R} \tag{5.64}$$

such that

$$\log(M(z)) = C + \int_{\mathbb{R}} d\lambda\, \widehat{\Xi}(\lambda)((\lambda - z)^{-1} - \lambda(1 + \lambda^2)^{-1}), \quad z \in \mathbb{C}_+ \tag{5.65}$$

the integral taken in the weak sense, where $C = C^* = \mathrm{Re}(\log(M(i))) \in \mathcal{B}(\mathcal{H})$. Moreover, suppose there exists a measurable subset $\Lambda \in \mathbb{R}$, $|\Lambda| \neq 0$ such that

$$\text{n-}\lim_{\varepsilon\to 0} M(\lambda + i\varepsilon) = M(\lambda + i0) \in \mathcal{B}(\mathcal{H}) \text{ for a.e. } \lambda \in \Lambda \tag{5.66}$$

such that $\mathrm{Im}(M(\lambda + i0)) \geq 0$ and $M(\lambda + i0)^{-1} \in \mathcal{B}(\mathcal{H})$ for a.e. $\lambda \in \Lambda$. Then

$$\widehat{\Xi}(\lambda) = \Xi(M(\lambda + i0)) \text{ for a.e. } \lambda \in \Lambda. \tag{5.67}$$

Proof. Since (5.64) and (5.65) have been proven in [19], we focus on (5.67). Let $\{P_n\}_{n\in\mathbb{N}}$ be an increasing family of orthogonal projections of rank n, that is, $\mathrm{rank}(P_n) = n$, $P_n\mathcal{H} \subset P_{n+1}\mathcal{H}$, with

$$\text{s-}\lim_{n\to\infty} P_n = I_{\mathcal{H}}. \tag{5.68}$$

Combining the norm continuity of the logarithm of bounded dissipative operators as discussed in Section 2 of [19] with the exponential Herglotz representation for $P_n \log(M(z))P_n$ (i.e., the finite-dimensional analog of (5.65) as in (5.15)–(5.17)), one infers for each $n \in \mathbb{N}$ the existence of a subset $\Lambda_n \subseteq \Lambda$, $|\Lambda\backslash\Lambda_n| = 0$ such that

$$P_n\widehat{\Xi}(\lambda)P_n = P_n\Xi(M(\lambda + i0))P_n \text{ for all } \lambda \in \Lambda_n. \tag{5.69}$$

Thus,

$$P_n\widehat{\Xi}(\lambda)P_n = P_n\Xi(M(\lambda + i0))P_n \text{ for all } \lambda \in \bigcap_{m\in\mathbb{N}} \Lambda_m,\ n \in \mathbb{N}. \tag{5.70}$$

Since $|\Lambda\backslash \bigcap_{n\in\mathbb{N}} \Lambda_n| = 0$ one concludes (5.67). ☐

Next, assuming H_0 and V to be self-adjoint operators in $\mathcal{H}$ with corresponding domains $\mathrm{dom}(H_0)$ and $\mathrm{dom}(V)$, such that

$$\mathrm{dom}(|V|^{1/2}) \supseteq \mathrm{dom}(|H_0|^{1/2}), \tag{5.71}$$

and introducing the signature operator

$$J = \mathrm{sgn}(V) \text{ with } J|_{\ker(V)} = I_{\mathcal{H}}|_{\ker(V)}, \tag{5.72}$$

we may define the bounded operator-valued Herglotz function $\phi(z) \in \mathcal{B}(\mathcal{H})$

$$\phi(z) = J + \overline{|V|^{1/2}(H_0 - z)^{-1}|V|^{1/2}}, \quad z \in \mathbb{C}_+. \tag{5.73}$$

(here the bar denotes the operator closure in $\mathcal{H}$.) In addition, we suppose that

$$\phi(z)^{-1} \in \mathcal{B}(\mathcal{H}) \text{ for some (and hence for all) } z \in \mathbb{C}_+. \tag{5.74}$$

Applying Theorem 5.8, one concludes that $\phi(z)$ admits the representation

$$\log(\phi(z)) = C + \int_{\mathbb{R}} d\lambda\, \widehat{\Xi}(\lambda, H_0, H)((\lambda - z)^{-1} - \lambda(1 + \lambda^2)^{-1}), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{5.75}$$

$$C = C^* = \mathrm{Re}(\log \phi(i)), \quad 0 \leq \widehat{\Xi}(\lambda, H_0, H) \leq I_{\mathcal{H}} \text{ for a.e. } \lambda \in \mathbb{R}. \tag{5.76}$$

Here our notation $\widehat{\Xi}(\lambda, H_0, H)$ emphasizes the underlying pair (H_0, H), where H"="$H_0 + V$ formally represents the perturbation of H_0 by V. We will return to a discussion of this point in Remark 5.10 below.

Definition 5.9. In addition to (5.71)–(5.76) assume the existence of a (Lebesgue) measurable set Λ, $|\Lambda| \neq 0$, such that the pair $(\widehat{\Xi}(\lambda, H_0, H), \Xi(J))$ has a trindex for a.e. $\lambda \in \Lambda$. Then the *generalized spectral shift function* $\widehat{\xi}(\cdot, H_0, H)$ associated with the pair (H_0, H) is defined by

$$\widehat{\xi}(\lambda, H_0, H) = \mathrm{trindex}(\widehat{\Xi}(\lambda, H_0, H), \Xi(J)) \text{ for a.e. } \lambda \in \Lambda. \tag{5.77}$$

Remark 5.10. A close look at $\phi(z)$ and $\widehat{\Xi}$ in (5.75) and (5.76) reveals that both objects depend on the self-adjoint operators H_0 and V. Thus, a logical choice of notation for $\widehat{\Xi}$ would have indicated its dependence on the pair (H_0, V). We decided against that choice since in practical applications, $\widehat{\Xi}$ in (5.75) is associated with a pair of self-adjoint operators (H_0, H), where H results as an additive perturbation of H_0 by V and hence resorted to the more familiar notation $\widehat{\Xi}(\lambda, H_0, H)$. But this raises the question of how to define such a self-adjoint operator H, given H_0 and V. Perhaps the most natural solution of this problem in our context goes back to Kato [26] (see also [28]) and proceeds as follows. One defines the resolvent of the self-adjoint operator H in $\mathcal{H}$ (and hence H itself) by

$$\begin{aligned}(H - z)^{-1} &= (H_0 - z)^{-1} \\ &\quad - (|V|^{1/2}(H_0 - \overline{z})^{-1})^* \phi(z)^{-1} \overline{|V|^{1/2}(H_0 - z)^{-1}}, \quad z \in \mathbb{C}_+.\end{aligned} \tag{5.78}$$

A detailed discussion of this point of view can be found in Yafaev's monograph [53, Sects. 1.9, 1.10].

By Theorem 5.3, the generalized spectral shift function coincides with Krein's spectral shift function in the case of trace class perturbations, that is,

$$\widehat{\xi}(\lambda, H_0, H) = \xi(\lambda, H_0, H) \text{ for a.e. } \lambda \in \mathbb{R}, \tag{5.79}$$

using the standard factorization of $(H - H_0)$ into $(H - H_0) = |V|^{1/2}\mathrm{sgn}(V)|V|^{1/2} \in \mathcal{B}_1(\mathcal{H})$.

Lemma 5.11. *Let S be a signature operator, $S = S^* = S^{-1}$, $A = A^* \in \mathcal{B}_\infty(\mathcal{H})$, and $\Lambda = \mathbb{R}\backslash\{\mathrm{spec}(S + A) \cup \{-1, 1\}\}$. Then the generalized spectral shift function $\widehat{\xi}(\lambda, S + A, S)$ associated with the pair $(S + A, S)$ is well-defined for a.e. $\lambda \in \Lambda$. Moreover, $\widehat{\xi}(\lambda, S + A, S)$ has a continuous representative on* Λ (still denoted by $\widehat{\xi}(\lambda, S + A, S)$) such that

$$\widehat{\xi}(\lambda, S + A, S) = \mathrm{index}(E_{S+A}((-\infty, \lambda)), E_S((-\infty, \lambda))), \quad \lambda \in \Lambda. \tag{5.80}$$

In particular, taking $\lambda \uparrow 0$,

$$\widehat{\xi}(0_-, S + A, S) = \mathrm{index}(E_{S+A}((-\infty, 0)), E_S((-\infty, 0))), \quad \lambda \in \Lambda. \tag{5.81}$$

Proof. Since $\mathrm{spec}(S) \subseteq \{-1, 1\}$ and $A \in \mathcal{B}_\infty(\mathcal{H})$, the spectrum of $S + A$ is a discrete set with only possible accumulation points at ± 1. Next, the normal boundary values

$|A|^{1/2}(S+A-\lambda+i0)^{-1}|A|^{1/2} = |A|^{1/2}(S+A-\lambda)^{-1}|A|^{1/2}$ exist in norm for all $\lambda \in \Lambda$. Moreover,

$$(\operatorname{sgn}(-A) + |A|^{1/2}(S+A-\lambda)^{-1}|A|^{1/2})^{-1} \in \mathcal{B}(\mathcal{H}), \quad \lambda \in \Lambda, \tag{5.82}$$

which can be seen as follows: suppose that (5.82) is false, then by compactness of A there exists an $f \in \mathcal{H}$ such that

$$(\operatorname{sgn}(-A) + |A|^{1/2}(S+A-\lambda)^{-1}|A|^{1/2})f = 0. \tag{5.83}$$

Multiplying (5.83) by $\operatorname{sgn}(-A)$ one infers that

$$(I_{\mathcal{H}} + \operatorname{sgn}(-A)|A|^{1/2}(S+A-\lambda)^{-1}|A|^{1/2})f = 0. \tag{5.84}$$

Since $A \in \mathcal{B}_\infty(\mathcal{H})$ and $\operatorname{spec}(CD)\backslash\{0\} = \operatorname{spec}(DC)\backslash\{0\}$ for any $C, D \in \mathcal{B}(\mathcal{H})$, one concludes that there is a $g \in \mathcal{H}$ such that $(I_{\mathcal{H}} - (S+A-\lambda)^{-1}A)g = 0$. Thus, $(S-\lambda)g = 0$ and hence $\lambda \in \{-1, 1\}$, which contradicts the fact that $\lambda \in \Lambda$. This proves (5.82).

By Theorem 5.8,

$$\widehat{\Xi}(\lambda, S+A, S) = \Xi(\operatorname{sgn}(-A) + |A|^{1/2}(S+A-\lambda)^{-1}|A|^{1/2}) \quad \text{for a.e. } \lambda \in \Lambda. \tag{5.85}$$

Moreover, the pair

$$(\operatorname{sgn}(-A) + |A|^{1/2}(S+A-\lambda)^{-1}|A|^{1/2}, \operatorname{sgn}(-A)) \tag{5.86}$$

is a Fedholm pair. Hence the generalized spectral shift function is well-defined and given by

$$\begin{aligned}\widehat{\xi}(\lambda, S+A, S) &= \operatorname{trindex}(\Xi(\operatorname{sgn}(-A) + |A|^{1/2}(S+A-\lambda)^{-1}|A|^{1/2}), \Xi(-A)) \\ &= \operatorname{index}(E_{\operatorname{sgn}(-A)+|A|^{1/2}(S+A-\lambda)^{-1}|A|^{1/2}}((-\infty,0)), E_{\operatorname{sgn}(-A)}((-\infty,0))) \\ &\qquad \text{for a.e. } \lambda \in \Lambda.\end{aligned} \tag{5.87}$$

Since the right-hand side of (5.87) is continuous on Λ by Theorem 3.12, $\widehat{\xi}(\lambda, S+A, S)$ has a continuous representative on Λ.

Next, assume $A \in \mathcal{B}_1(\mathcal{H})$. Then Krein's spectral shift function $\xi(\lambda, S+A, S)$ associated with the pair $(S+A, S)$ coincides with the right-hand side of (5.80) for a.e. $\lambda \in \mathbb{R}$ (see, e.g., [8]), proving (5.80) for $A \in \mathcal{B}_1(\mathcal{H})$ applying (5.79).

The general case of compact operators $A \in \mathcal{B}_\infty(\mathcal{H})$ can be handled using an appropriate approximation argument. Denoting by $\{\lambda_n\}_{n\in\mathbb{Z}}$ the eigenvalues of A and by $\{P_n\}_{n\in\mathbb{Z}}$ the corresponding spectral projections associated with λ_n, and introducing the family of the self-adjoint operators

$$A_\rho = \sum_{n\in\mathbb{Z}} \rho^{-|n|}\lambda_n P_n, \quad \rho \in (0,1), \tag{5.88}$$

one concludes that $A_\rho \in \mathcal{B}_1(\mathcal{H})$, $\rho \in (0,1)$, and

$$\operatorname*{n-lim}_{\rho\uparrow 1} \|A_\rho - A\| = 0. \tag{5.89}$$

Given $\lambda \in \Lambda$, there exists a $\rho_0 \in (0,1)$, such that for all $\rho \in (\rho_0, 1)$ the point $\lambda \in \Lambda_\rho$, $\Lambda_\rho = \mathbb{R}\backslash\{\operatorname{spec}(S+A_\rho) \cup \{-1,1\}\}$, and therefore, by (5.80) (for $A \in \mathcal{B}_1(\mathcal{H})$), for such ρ we have the representation

$$\xi(\lambda, S+A_\rho, S) = \operatorname{index}(E_{S+A_\rho}((-\infty,\lambda)), E_S((-\infty,\lambda))), \quad \rho \in (\rho_0, 1). \tag{5.90}$$

Here $\xi(\lambda, S+A_\rho, S)$ denotes the continuous representative of (the piecewise constant) Krein's spectral shift function on Λ_ρ.

Applying Theorem 3.12 once again, one can pass to the limit $\rho \uparrow 1$ to obtain

$$\lim_{\rho\uparrow 1} \xi(\lambda, S + A_\rho, S) = \operatorname{index}(E_{S+A}((-\infty, \lambda)), E_S((-\infty, \lambda)), \quad \lambda \in \Lambda. \tag{5.91}$$

By (5.87) we also have

$$\begin{aligned} &\xi(\lambda, S + A_\rho, S) \\ &= \operatorname{index}(E_{\operatorname{sgn}(-A_\rho)+|A_\rho|^{1/2}(S+A_\rho-\lambda)^{-1}|A_\rho|^{1/2}}((-\infty, 0)), E_{\operatorname{sgn}(-A_\rho)}((-\infty, 0))). \end{aligned} \tag{5.92}$$

Taking into account that $\operatorname{sgn}(-A_\rho) = \operatorname{sgn}(-A)$, $\rho \in (0, 1)$ (5.92) implies

$$\begin{aligned} &\lim_{\rho\uparrow 1} \xi(\lambda, S + A_\rho, S) \\ &= \operatorname{index}(E_{\operatorname{sgn}(-A)+|A|^{1/2}(S+A-\lambda)^{-1}|A|^{1/2}}((-\infty, 0)), E_{\operatorname{sgn}(-A)}((-\infty, 0))), \quad \lambda \in \Lambda \end{aligned} \tag{5.93}$$

by Theorem 3.12. The right-hand side of (5.93) coincides with the continuous representative of the generalized spectral shift function $\widehat{\xi}(\lambda, S+A, S)$, $\lambda \in \Lambda$, which together with (5.91) proves (5.80). Finally, (5.81) is a consequence of (5.80) and the left continuity of $\operatorname{index}(E_{S+A}((-\infty, \lambda)), E_S((-\infty, \lambda)))$ on $\mathbb{R} \setminus \{-1, 1\}$. □

Combining Theorem 5.5 and Lemma 5.11, one can finally reformulate Theorem 5.5 as follows using the concept of the generalized spectral shift function.

Theorem 5.12. *Under the assumptions of Theorem* 5.5*, the spectral shift function* $\widehat{\xi}(\lambda, H_0, H)$ *associated with the pair* (H_0, H) *admits the representation*

$$\widehat{\xi}(\lambda, H_0, H) = \frac{1}{\pi} \int_{\mathbb{R}} dt\, \frac{\widehat{\xi}(0_-, J + A(\lambda) + tB(\lambda), J)}{1 + t^2}, \text{ for a.e. } \lambda \in \mathbb{R}, \tag{5.94}$$

where $\widehat{\xi}(\cdot, J + A(\lambda) + tB(\lambda), J)$ *is the continuous representative of the generalized spectral shift function associated with the pair* $(J + A(\lambda) + tB(\lambda), J)$ *for a.e.* $\lambda \in \mathbb{R}$*,* $t \in \mathbb{R}$*.*

Proof. The assertion is a direct consequence of Theorem 5.5 and Lemma 5.11. □

Remark 5.13. Suppose H, H_0, V are self-adjoint in $\mathcal{H}$, with $V \in \mathcal{B}_1(\mathcal{H})$ and $H = H_0 + V$. Suppose H_0 has a spectral gap and $\lambda \in \Lambda$, with Λ a joint spectral gap of H_0 and H. Then (5.94) turns into

$$\xi(\lambda, H_0, H) = \xi(0, J + |V|^{1/2}(H_0 - \lambda)^{-1}|V|^{1/2}, J), \quad \lambda \in \Lambda, \tag{5.95}$$

where $\xi(\lambda, H_0, H)$ ($\xi(0, J + |V|^{1/2}(H_0 - \lambda)^{-1}|V|^{1/2}, J)$) denotes the continuous representative of Krein's spectral shift function associated with the pair (H_0, H) ($(J + |V|^{1/2}(H_0 - \lambda)^{-1}|V|^{1/2}, J)$) on Λ. In particular, if H_0 is bounded from below and $\lambda < \inf(H_0)$, and the perturbation V is non-positive (i.e., $V \le 0$), the equality (5.95) has the following meaning: the number of eigenvalues of the operator $H = H_0 + V$, located to the left of the point λ, $\lambda < \inf(H_0)$, coincides with the number of eigenvalues of $|V|^{1/2}(H_0 - \lambda)^{-1}|V|^{1/2}$ which are greater than 1. Therefore, in this special case where $\lambda < \inf \operatorname{spec}(H_0)$, (5.95) represents the classical *Birman–Schwinger principle* (a term coined by Simon, see, e.g., [47]) as originally introduced by Birman [5] (see also [46, Ch. 7]). Thus, (5.95) should be interpreted as the *Birman-Schwinger principle in a gap* and hence (5.94) as the *generalized Birman-Schwinger principle.* We emphasize that Theorem 5.12 introduces a new twist in connection with the (generalized) Birman-Schwinger principle: the role of eigenvalue counting functions in the traditional formulation of the Birman-Schwinger principle (see [10] for a modern formulation of the principle) is now replaced by the more general concept of the (generalized) spectral shift function $\widehat{\xi}(\lambda, H_0, H)$ and an appropriate average over $\widehat{\xi}(0_-, J + A(\lambda) + tB(\lambda), J)$.

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Department of Mathematics, University of Missouri, Columbia, MO 65211, USA
E-mail address: `fritz@math.missouri.edu`
URL: `http://www.math.missouri.edu/people/fgesztesy.html`

Department of Mathematics, University of Missouri, Columbia, MO 65211, USA
E-mail address: makarov@azure.math.missouri.edu
URL: http://www.math.missouri.edu/people/kmakarov.html