SOME APPLICATIONS OF THE SPECTRAL SHIFT OPERATOR

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Abstract. The recently introduced concept of a spectral shift operator is applied in several instances. Explicit applications include Krein's trace formula for pairs of self-adjoint operators, the Birman-Solomyak spectral averaging formula and its operator-valued extension, and an abstract approach to trace formulas based on perturbation theory and the theory of self-adjoint extensions of symmetric operators.

1. Introduction

The concept of a spectral shift function, historically first introduced by I. M. Lifshits [51], [52] and then developed into a powerful spectral theoretic tool by M. Krein [47], [48], [50], attracted considerable attention in the past due to its widespread applications in a variety of fields including 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. For an extensive bibliography in this connection we refer to [33]; detailed reviews on the spectral shift function and its applications were published by Birman and Yafaev [11], [12] in 1993.

The principal aim of this paper is to follow up on our recent paper [33], which was devoted to the introduction of a spectral shift operator $\Xi(\lambda, H_0, H)$ for a.e. $\lambda \in \mathbb{R}$, associated with a pair of self-adjoint operators H_0, $H = H_0 + V$ with $V \in \mathcal{B}_1(\mathcal{H})$ ($\mathcal{H}$ a complex separable Hilbert space). In the special cases of sign-definite perturbations $V \geq 0$ and $V \leq 0$, $\Xi(\lambda, H_0, H)$ turns out to be a trace class operator in $\mathcal{H}$, whose trace coincides with Krein's spectral shift function $\xi(\lambda, H_0, H)$ for the pair (H_0, H). While the special case $V \geq 0$ has previously been studied by Carey [15], our aim in [33] was to treat the case of general interactions V by separately introducing the positive and negative parts $V_\pm = (|V| \pm V)/2$ of V. In general, if V is not sign-definite, then $\Xi(\lambda, H_0, H)$ (naturally associated with (3.5)) is not necessarily of trace class. However, we introduced trace class operators $\Xi_\pm(\lambda)$ corresponding to $V_\pm$, acting in distinct Hilbert spaces $\mathcal{H}_\pm$, such that

$$\xi(\lambda, H_0, H) = \mathrm{tr}_{\mathcal{H}_+}(\Xi_+(\lambda)) - \mathrm{tr}_{\mathcal{H}_-}(\Xi_-(\lambda)) \text{ for a.e. } \lambda \in \mathbb{R}. \tag{1.1}$$

(An alternative approach to $\xi(\lambda, H_0, H)$, which does not rely on separately introducing V_+ and V_-, will be discussed elsewhere [32].)

Our main techniques are based on operator-valued Herglotz functions (continuing some of our recent investigations in this area [31], [34], [36]) and especially, on a detailed study of logarithms of Herglotz operators in Section 2 following the treatment in [33]. In Section 3 we introduce the spectral shift operator $\Xi(\lambda, H_0, H)$ associated

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with the pair (H_0, H) and relate it to Krein's spectral shift function $\xi(\lambda, H_0, H)$ and his celebrated trace formula [47]. Finally, Section 4 provides various applications of this formalism including spectral averaging originally due to Birman and Solomyak [10], its operator-valued generalization first discussed in [33], connections with the scattering operator, and an abstract version of a trace formula, combining perturbation theory and the theory of self-adjoint extensions.

2. Logarithms of Operator-Valued Herglotz Functions

The principal purpose of this section is to recall the basic properties of logarithms and associated representation theorems for operator-valued Herglotz functions following the treatment in [33].

In the following $\mathcal{H}$ denotes a complex separable Hilbert space with scalar product $(\cdot,\cdot)_{\mathcal{H}}$ (linear in the second factor) and norm $||\cdot||_{\mathcal{H}}$, $I_{\mathcal{H}}$ the identity operator in $\mathcal{H}$, $\mathcal{B}(\mathcal{H})$ the Banach space of bounded linear operators defined on $\mathcal{H}$, $\mathcal{B}_p(\mathcal{H})$, $p \geq 1$ the standard Schatten-von Neumann ideals of $\mathcal{B}(\mathcal{H})$ (cf., e.g., [37], [62]) and $\mathbb{C}_+$ (respectively, $\mathbb{C}_-$) the open complex upper (respectively, lower) half-plane. Moreover, real and imaginary parts of a bounded operator $T \in \mathcal{B}(\mathcal{H})$ are defined as usual by $\operatorname{Re}(T) = (T + T^*)/2$, $\operatorname{Im}(T) = (T - T^*)/(2i)$.

Definition 2.1. $M : \mathbb{C}_+ \to \mathcal{B}(\mathcal{H})$ is called an *operator-valued Herglotz function* (in short, a *Herglotz operator*) if M is analytic on $\mathbb{C}_+$ and $\operatorname{Im}(M(z)) \geq 0$ for all $z \in \mathbb{C}_+$.

Theorem 2.2. (Birman and Entina [7], de Branges [22], Naboko [53]–[55].) *Let $M : \mathbb{C}_+ \to \mathcal{B}(\mathcal{H})$ be a Herglotz operator.*
(i) Then there exist bounded self-adjoint operators $A = A^* \in \mathcal{B}(\mathcal{H})$, $0 \leq B \in \mathcal{B}(\mathcal{H})$, a Hilbert space $\mathcal{K} \supseteq \mathcal{H}$, a self-adjoint operator $L = L^*$ in $\mathcal{K}$, a bounded nonnegative operator $0 \leq R \in \mathcal{B}(\mathcal{K})$ with $R|_{\mathcal{K}\ominus\mathcal{H}} = 0$ such that

$$M(z) = A + Bz + R^{1/2}(I_{\mathcal{K}} + zL)(L - z)^{-1}R^{1/2}|_{\mathcal{H}} \tag{2.1a}$$

$$= A + (B + R|_{\mathcal{H}})z + (1 + z^2)R^{1/2}(L - z)^{-1}R^{1/2}|_{\mathcal{H}}. \tag{2.1b}$$

(ii) Let $p \geq 1$. Then $M(z) \in \mathcal{B}_p(\mathcal{H})$ for all $z \in \mathbb{C}_+$ if and only if $M(z_0) \in \mathcal{B}_p(\mathcal{H})$ for some $z_0 \in \mathbb{C}_+$. In this case necessarily $A, B, R \in \mathcal{B}_p(\mathcal{H})$.
(iii) Let $M(z) \in \mathcal{B}_1(\mathcal{H})$ for some (and hence for all) $z \in \mathbb{C}_+$. Then $M(z)$ has normal boundary values $M(\lambda + i0)$ for (Lebesgue) a.e. $\lambda \in \mathbb{R}$ in every $\mathcal{B}_p(\mathcal{H})$-norm, $p > 1$. Moreover, let $\{E_L(\lambda)\}_{\lambda\in\mathbb{R}}$ be the family of orthogonal spectral projections of L in $\mathcal{K}$. Then $R^{1/2}E_L(\lambda)R^{1/2}$ is $\mathcal{B}_1(\mathcal{H})$-differentiable for a.e. $\lambda \in \mathbb{R}$ and denoting the derivative by $d(R^{1/2}E_L(\lambda)R^{1/2})/d\lambda$, $\operatorname{Im}(M(z))$ has normal boundary values $\operatorname{Im}(M(\lambda + i0))$ for a.e. $\lambda \in \mathbb{R}$ in $\mathcal{B}_1(\mathcal{H})$-norm given by

$$\lim_{\varepsilon\downarrow 0} ||\pi^{-1}\operatorname{Im}(M(\lambda + i\varepsilon)) - d(R^{1/2}E_L(\lambda)R^{1/2}|_{\mathcal{H}})/d\lambda||_{\mathcal{B}_1(\mathcal{H})} = 0 \ \text{a.e.} \tag{2.2}$$

Originally, the existence of normal limits $M(\lambda + i0)$ for a.e. $\lambda \in \mathbb{R}$ in $\mathcal{B}_2(\mathcal{H})$-norm, in the special case $A = 0$, $B = -R|_{\mathcal{H}}$, assuming $M(z) \in \mathcal{B}_1(\mathcal{H})$, was proved by de Branges [22] in 1962. (The more general case in (2.1) can easily be reduced to this special case.) In his paper [22], de Branges also proved the existence of normal limits $\operatorname{Im}(M(\lambda + i0))$ for a.e. $\lambda \in \mathbb{R}$ in $\mathcal{B}_1(\mathcal{H})$-norm and obtained (2.2). These results and their implications on stationary scattering theory were subsequently studied in detail by Birman and Entina [6], [7]. (Textbook representations of this material can also be found in [4], Ch. 3.)

Invoking the family of orthogonal spectral projections $\{E_L(\lambda)\}_{\lambda\in\mathbb{R}}$ of L, (2.1) then yields the familiar representation

(2.3)
$$M(z) = A + Bz + \int_{\mathbb{R}} (1+\lambda^2) d(R^{1/2}E_L(\lambda)R^{1/2}|_{\mathcal{H}})((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}),$$

where for our purpose it suffices to interpret the integral in (2.3) in the weak sense. Further results on representations of the type (2.3) can be found in [13], Sect. I.4 and [61].

Since we are interested in logarithms of Herglotz operators, questions of their invertibility naturally arise. The following result clarifies the situation.

Lemma 2.3. ([33].) *Suppose M is a Herglotz operator with values in $\mathcal{B}(\mathcal{H})$. If $M(z_0)^{-1} \in \mathcal{B}(\mathcal{H})$ for some $z_0 \in \mathbb{C}_+$ then $M(z)^{-1} \in \mathcal{B}(\mathcal{H})$ for all $z \in \mathbb{C}_+$.*

Concerning boundary values at the real axis we also recall

Lemma 2.4. (Naboko [56].) *Suppose $(M - I_{\mathcal{H}})$ is a Herglotz operator with values in $\mathcal{B}_1(\mathcal{H})$. Then the boundary values $M(\lambda+i0)$ exist for a.e. $\lambda \in \mathbb{R}$ in $\mathcal{B}_p(\mathcal{H})$-norm, $p > 1$ and $M(\lambda + i0)$ is a Fredholm operator for a.e. $\lambda \in \mathbb{R}$ with index zero a.e.,*

$$\operatorname{ind}(M(\lambda + i0)) = 0 \text{ for a.e. } \lambda \in \mathbb{R}. \tag{2.4}$$

Moreover,

$$\ker(M(\lambda + i0)) = \ker(M(i)) = (\operatorname{ran}(M(\lambda + i0)))^{\perp} \text{ for a.e. } \lambda \in \mathbb{R}. \tag{2.5}$$

In addition, if $M(z_0)^{-1} \in \mathcal{B}(\mathcal{H})$ for some (and hence for all) $z_0 \in \mathbb{C}_+$, then

$$M(\lambda + i0)^{-1} \in \mathcal{B}(\mathcal{H}) \text{ for a.e. } \lambda \in \mathbb{R}. \tag{2.6}$$

Next, let T be a bounded *dissipative* operator, that is,

$$T \in \mathcal{B}(\mathcal{H}), \quad \operatorname{Im}(T) \geq 0. \tag{2.7}$$

In order to define the logarithm of T we use the integral representation

$$\log(z) = -i \int_0^\infty d\lambda \, ((z + i\lambda)^{-1} - (1 + i\lambda)^{-1}), \quad z \neq -iy, \, y \geq 0, \tag{2.8}$$

with a cut along the negative imaginary z-axis. We use the symbol $\log(\cdot)$ in (2.8) in order to distinguish it from the integral representation

$$\ln(z) = \int_{-\infty}^0 d\lambda \, ((\lambda - z)^{-1} - \lambda(1 + \lambda^2)^{-1}), \quad z \in \mathbb{C}\backslash(-\infty, 0] \tag{2.9}$$

with a cut along the negative real axis. It is easily verified that $\log(\cdot)$ and $\ln(\cdot)$ coincide for $z \in \mathbb{C}_+$. In particular, one verifies that (2.8) and (2.9) are Herglotz functions, that is, they are analytic in $\mathbb{C}_+$ and

$$0 < \operatorname{Im}(\log(z)), \ \operatorname{Im}(\ln(z)) < \pi, \quad z \in \mathbb{C}_+. \tag{2.10}$$

Lemma 2.5. ([33].) *Suppose $T \in \mathcal{B}(\mathcal{H})$ is dissipative and $T^{-1} \in \mathcal{B}(\mathcal{H})$. Define*

$$\log(T) = -i \int_0^\infty d\lambda \, ((T + i\lambda)^{-1} - (1 + i\lambda)^{-1} I_{\mathcal{H}}) \tag{2.11}$$

in the sense of a $\mathcal{B}(\mathcal{H})$-norm convergent Riemann integral. Then
(i) $\log(T) \in \mathcal{B}(\mathcal{H})$.
(ii) If $T = zI_{\mathcal{H}}$, $z \in \mathbb{C}_+$, then $\log(T) = \log(z) I_{\mathcal{H}}$.

(iii) Suppose $\{P_n\}_{n\in\mathbb{N}} \subset \mathcal{B}(\mathcal{H})$ *is a family of orthogonal finite-rank projections in* $\mathcal{H}$ *with* $\text{s-lim}_{n\to\infty} P_n = I_{\mathcal{H}}$. *Then*

$$\operatorname*{s-lim}_{n\to\infty}((I_{\mathcal{H}} - P_n) + P_n T P_n) = T$$

and

$$\begin{aligned}&\operatorname*{s-lim}_{n\to\infty} \log((I_{\mathcal{H}} - P_n) + P_n(T + i\varepsilon)P_n) \\ &= \operatorname*{s-lim}_{n\to\infty} P_n(\log(P_n(T+i\varepsilon)P_n|_{P_n\mathcal{H}})P_n = \log(T + i\varepsilon I_H), \quad \varepsilon > 0.\end{aligned}$$

(iv) $\text{n-lim}_{\varepsilon\downarrow 0} \log(T + i\varepsilon I_{\mathcal{H}}) = \log(T)$.
(v) $e^{\log(T)} = T$.

Lemma 2.6. ([33].) *Suppose* $T \in \mathcal{B}(\mathcal{H})$ *is dissipative and* $T^{-1} \in \mathcal{B}(\mathcal{H})$. *Let* L *be the minimal self-adjoint dilation of* T *in the Hilbert space* $\mathcal{K} \supseteq \mathcal{H}$. *Then*

$$\operatorname{Im}(\log(T)) = \pi P_{\mathcal{H}} E_L((-\infty, 0))|_{\mathcal{H}}, \tag{2.12}$$

where $P_{\mathcal{H}}$ *is the orthogonal projection in* $\mathcal{K}$ *onto* $\mathcal{H}$ *and* $\{E_L(\lambda)\}_{\lambda\in\mathbb{R}}$ *is the family of orthogonal spectral projections of* L *in* $\mathcal{K}$. *In particular,*

$$0 \le \operatorname{Im}(\log(T)) \le \pi I_{\mathcal{H}}. \tag{2.13}$$

Combining Lemmas 2.3 and 2.6 one obtains the following result.

Lemma 2.7. ([33].) *Suppose* $M : \mathbb{C}_+ \longrightarrow \mathcal{B}(\mathcal{H})$ *is a Herglotz operator and assume that* $M(z_0)^{-1} \in \mathcal{B}(\mathcal{H})$ *for some (and hence for all)* $z_0 \in \mathbb{C}_+$. *Then* $\log(M) : \mathbb{C}_+ \longrightarrow \mathcal{B}(\mathcal{H})$ *is a Herglotz operator and*

$$0 \le \operatorname{Im}(\log(M(z))) \le \pi I_{\mathcal{H}}, \quad z \in \mathbb{C}_+. \tag{2.14}$$

Theorem 2.8. ([33].) *Suppose* $M : \mathbb{C}_+ \longrightarrow \mathcal{B}(\mathcal{H})$ *is a Herglotz operator 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* $\{\Xi(\lambda)\}_{\lambda\in\mathbb{R}} \subset \mathcal{B}(\mathcal{H})$,

$$0 \le \Xi(\lambda) \le I_{\mathcal{H}} \text{ for a.e. } \lambda \in \mathbb{R} \tag{2.15}$$

such that

$$\log(M(z)) = C + \int_{\mathbb{R}} d\lambda\, \Xi(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \quad z \in \mathbb{C}_+ \tag{2.16}$$

the integral taken in the weak sense, where $C = C^* \in \mathcal{B}(\mathcal{H})$. *Moreover, if* $\operatorname{Im}(\log (M(z_0))) \in \mathcal{B}_1(\mathcal{H})$ *for some (and hence for all)* $z_0 \in \mathbb{C}_+$, *then*

$$0 \le \Xi(\lambda) \in \mathcal{B}_1(\mathcal{H}) \text{ for a.e. } \lambda \in \mathbb{R}, \tag{2.17}$$

$$0 \le \operatorname{tr}_{\mathcal{H}}(\Xi(\cdot)) \in L^1_{\text{loc}}(\mathbb{R}; d\lambda), \quad \int_{\mathbb{R}} d\lambda\, (1+\lambda^2)^{-1} \operatorname{tr}_{\mathcal{H}}(\Xi(\lambda)) < \infty, \tag{2.18}$$

and

$$\operatorname{tr}_{\mathcal{H}}(\operatorname{Im}(\log(M(z)))) = \operatorname{Im}(z) \int_{\mathbb{R}} d\lambda\, \operatorname{tr}_{\mathcal{H}}(\Xi(\lambda))|\lambda - z|^{-2}, \quad z \in \mathbb{C}_+. \tag{2.19}$$

Remark 2.9. For simplicity we only focused on dissipative operators. Later we will also encounter operators $S \in \mathcal{B}(\mathcal{H})$ with $-S$ dissipative, that is, $\operatorname{Im}(S) \le 0$ (cf. (3.13b)). In this case S^* is dissipative and one can simply define $\log(S)$ by

$$\log(S) = (\log(S^*))^*, \tag{2.20}$$

with $\log(S^*)$ defined as in (2.11). Moreover,

$$\log(\widehat{M}(z)) = \widehat{C} - \int_{\mathbb{R}} d\lambda \, \widehat{\Xi}(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \quad z \in \mathbb{C}_+, \tag{2.21}$$

$$\widehat{C} = \widehat{C}^* \in \mathcal{B}(\mathcal{H}) \text{ and } 0 \le \widehat{\Xi}(\lambda) \le I_{\mathcal{H}} \text{ for a.e. } \lambda \in \mathbb{R}, \tag{2.22}$$

whenever $\widehat{M}$ is analytic in $\mathbb{C}_+$ and $\operatorname{Im}(\widehat{M}(z)) \le 0$, $z \in \mathbb{C}_+$.

Remark 2.10. Theorem 2.8 represents the operator-valued generalization of the exponential Herglotz representation for scalar Herglotz functions studied in detail by Aronszajn and Donoghue [2] (see also Carey and Pepe [16]). Prior to our proof of Theorem 2.8 in [33], Carey [15] considered the case $M(z) = I_{\mathcal{H}} + K^*(H_0 - z)^{-1}K$ in 1976 and established

$$M(z) = \exp\left(\int_{\mathbb{R}} d\lambda \, \Xi(\lambda)(\lambda - z)^{-1}\right) \tag{2.23}$$

for a summable operator function $\Xi(\lambda)$, $0 \le \Xi(\lambda) \le I_{\mathcal{H}}$. Carey's proof is different from ours and does not utilize the integral representation (2.11) for logarithms.

3. The Spectral Shift Operator

The main purpose of this section is to recall the concept of a spectral shift operator (cf. Definition 3.4) as developed in [33].

Suppose $\mathcal{H}$ is a complex separable Hilbert space and assume the following hypothesis for the remainder of this section.

Hypothesis 3.1. *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

$$V = KJK^* \tag{3.1}$$

we define the self-adjoint operator

$$H = H_0 + V, \quad \operatorname{dom}(H) = \operatorname{dom}(H_0) \tag{3.2}$$

in $\mathcal{H}$.

Given Hypothesis 3.1 we decompose $\mathcal{H}$ and J according to

$$J = \begin{pmatrix} I_+ & 0 \\ 0 & -I_- \end{pmatrix}, \quad \mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-, \tag{3.3}$$

$$J_+ = \begin{pmatrix} I_+ & 0 \\ 0 & 0 \end{pmatrix}, \quad J_- = \begin{pmatrix} 0 & 0 \\ 0 & I_- \end{pmatrix}, \quad J = J_+ - J_-, \tag{3.4}$$

with $I_\pm$ the identity operator in $\mathcal{H}_\pm$. Moreover, we introduce the following bounded operators

$$\Phi(z) = J + K^*(H_0 - z)^{-1}K : \mathcal{H} \to \mathcal{H}, \tag{3.5}$$

$$\Phi_+(z) = I_+ + J_+K^*(H_0 - z)^{-1}K|_{\mathcal{H}_+} : \mathcal{H}_+ \to \mathcal{H}_+, \tag{3.6}$$

$$\widetilde{\Phi}_-(z) = I_- - J_-K^*(H_+ - z)^{-1}K|_{\mathcal{H}_-} : \mathcal{H}_- \to \mathcal{H}_-, \tag{3.7}$$

for $z \in \mathbb{C}\backslash\mathbb{R}$, where

$$V_+ = KJ_+K^*, \tag{3.8}$$

$$H_+ = H_0 + V_+, \quad \mathrm{dom}(H_+) = \mathrm{dom}(H_0). \tag{3.9}$$

Lemma 3.2. ([33].) *Assume Hypothesis 3.1. Then* Φ, Φ_+, *and* $-\widetilde{\Phi}_-$ *are Herglotz operators in* $\mathcal{H}$, $\mathcal{H}_+$, *and* $\mathcal{H}_-$, *respectively. In addition* ($z \in \mathbb{C}\backslash\mathbb{R}$),

$$\Phi(z)^{-1} = J - JK^*(H-z)^{-1}KJ, \tag{3.10}$$

$$\Phi_+(z)^{-1} = I_+ - J_+K^*(H_+-z)^{-1}K|_{\mathcal{H}_+}, \tag{3.11}$$

$$\widetilde{\Phi}_-(z)^{-1} = I_- + J_-K^*(H-z)^{-1}K|_{\mathcal{H}_-}. \tag{3.12}$$

We also recall the following result (cf. [33]).

Lemma 3.3. *Assume Hypothesis 3.1 and* $\mathbb{C}\backslash\mathbb{R}$. *Then*

$$\mathrm{tr}_{\mathcal{H}}((H_0-z)^{-1} - (H_+-z)^{-1}) = d\,\mathrm{tr}_{\mathcal{H}_+}(\log(\Phi_+(z)))/dz, \tag{3.13a}$$

$$\mathrm{tr}_{\mathcal{H}}((H_+-z)^{-1} - (H-z)^{-1}) = d\,\mathrm{tr}_{\mathcal{H}_-}(\log(\widetilde{\Phi}_-(z)))/dz. \tag{3.13b}$$

Next, applying Theorem 2.8 and Remark 2.9 to $\Phi_+(z)$ and $\widetilde{\Phi}_-(z)$ one infers the existence of two families of bounded operators $\{\Xi_\pm(\lambda)\}_{\lambda\in\mathbb{R}}$ defined for (Lebesgue) a.e. $\lambda \in \mathbb{R}$ and satisfying

$$\begin{aligned} &0 \le \Xi_\pm(\lambda) \le I_\pm, \quad \Xi_\pm(\lambda) \in \mathcal{B}_1(\mathcal{H}_\pm) \text{ for a.e. } \lambda \in \mathbb{R}, \\ &||\Xi_\pm(\cdot)||_1 \in L^1(\mathbb{R}; (1+\lambda^2)^{-1}d\lambda) \end{aligned} \tag{3.14}$$

and

$$\begin{aligned} \log(\Phi_+(z)) &= \log(I_+ + J_+K^*(H_0-z)^{-1}K|_{\mathcal{H}_+}) \\ &= C_+ + \int_{\mathbb{R}} d\lambda\, \Xi_+(\lambda)((\lambda-z)^{-1} - \lambda(1+\lambda^2)^{-1}), \end{aligned} \tag{3.15a}$$

$$\begin{aligned} \log(\widetilde{\Phi}_-(z)) &= \log(I_- - J_-K^*(H_+-z)^{-1}K|_{\mathcal{H}_-}) \\ &= C_- - \int_{\mathbb{R}} d\lambda\, \Xi_-(\lambda)((\lambda-z)^{-1} - \lambda(1+\lambda^2)^{-1}) \end{aligned} \tag{3.15b}$$

for $z \in \mathbb{C}\backslash\mathbb{R}$, with $C_\pm = C_\pm^* \in \mathcal{B}_1(\mathcal{H})$.
Equations (3.15) motivate the following

Definition 3.4. $\Xi_+(\lambda)$ (respectively, $\Xi_-(\lambda)$) is called the *spectral shift operator* associated with $\Phi_+(z)$ (respectively, $\widetilde{\Phi}_-(z)$). Alternatively, we will refer to $\Xi_+(\lambda)$ as the spectral shift operator associated with the pair (H_0, H_+) and occasionally use the notation $\Xi_+(\lambda, H_0, H_+)$ to stress the dependence on (H_0, H_+), etc.

Moreover, we introduce

$$\xi_\pm(\lambda) = \mathrm{tr}_{\mathcal{H}_\pm}(\Xi_\pm(\lambda)), \quad 0 \le \xi_\pm \in L^1(\mathbb{R}; (1+\lambda^2)^{-1}d\lambda) \text{ for a.e. } \lambda \in \mathbb{R}. \tag{3.16}$$

Actually, taking into account the simple behavior of $\Phi_+(iy)$ and $\widetilde{\Phi}_-(iy)$ as $|y| \to \infty$, one can improve (3.15a) and (3.15b) as follows.

Lemma 3.5. ([33].) *Assume Hypothesis 3.1 and define* $\xi_\pm$ *as in* (3.16). *Then*

$$0 \le \xi_\pm \in L^1(\mathbb{R}; d\lambda), \tag{3.17}$$

and (3.15a) *and* (3.15b) *simplify to*

$$\log(\Phi_+(z)) = \int_{\mathbb{R}} d\lambda\, \Xi_+(\lambda)(\lambda-z)^{-1}, \tag{3.18a}$$

$$\log(\widetilde{\Phi}_-(z)) = -\int_{\mathbb{R}} d\lambda\, \Xi_-(\lambda)(\lambda - z)^{-1}. \tag{3.18b}$$

Moreover, for a.e. $\lambda \in \mathbb{R}$,

$$\lim_{\varepsilon\downarrow 0} \|\Xi_+(\lambda) - \pi^{-1}\mathrm{Im}(\log(\Phi_+(\lambda + i\varepsilon)))\|_{\mathcal{B}_1(\mathcal{H}_+)} = 0, \tag{3.19a}$$

$$\lim_{\varepsilon\downarrow 0} \|\Xi_-(\lambda) + \pi^{-1}\mathrm{Im}(\log(\widetilde{\Phi}_-(\lambda + i\varepsilon)))\|_{\mathcal{B}_1(\mathcal{H}_-)} = 0. \tag{3.19b}$$

Proof. For convenience of the reader we reproduce here the proof first presented in [33]. It suffices to consider $\xi_+(\lambda)$ and $\Phi_+(z)$. Since

$$\|\log(\Phi_+(y))\|_1 = O(|y|^{-1}) \text{ as } |y| \to \infty \tag{3.20}$$

by the Hilbert-Schmidt hypothesis on K and the fact $\|(H_0 - iy)^{-1}\| = O(|y|^{-1})$ as $|y| \to \infty$, the scalar Herglotz function $\mathrm{tr}_{\mathcal{H}_+}(\log(\Phi_+(z)))$ satisfies

$$|\,\mathrm{tr}_{\mathcal{H}_+}(\log(\Phi_+(z)))| = O(|y|^{-1}) \text{ as } |y| \to \infty. \tag{3.21}$$

By standard results (see, e.g., [2], [41]), (3.21) yields

$$\mathrm{tr}_{\mathcal{H}_+}(\log(\Phi_+(z))) = \int_{\mathbb{R}} d\omega_+(\lambda)(\lambda - z)^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{3.22}$$

where ω_+ is a finite measure,

$$\int_{\mathbb{R}} d\omega_+(\lambda) = -i \lim_{y\uparrow\infty}(y\,\mathrm{tr}_{\mathcal{H}_+}(\log(\Phi_+(z)))) < \infty. \tag{3.23}$$

Moreover, the fact that $\mathrm{Im}(\log(\Phi_+(z)))$ is uniformly bounded with respect to $z \in \mathbb{C}_+$ yields that ω_+ is purely absolutely continuous,

$$d\omega_+(\lambda) = \xi_+(\lambda)d\lambda, \quad \xi_+ \in L^1(\mathbb{R}; d\lambda), \tag{3.24}$$

where

$$\begin{aligned}\xi_+(\lambda) &= \pi^{-1}\lim_{\varepsilon\downarrow 0}(\mathrm{Im}(\mathrm{tr}_{\mathcal{H}_+}(\log(\Phi_+(\lambda + i\varepsilon))))) = \mathrm{tr}_{\mathcal{H}_+}(\Xi_+(\lambda)) \\ &= \pi^{-1}\lim_{\varepsilon\downarrow 0}(\mathrm{Im}(\log(\det_{\mathcal{H}_+}(\Phi_+(\lambda + i\varepsilon))))) \text{ for a.e. } \lambda \in \mathbb{R}.\end{aligned} \tag{3.25}$$

In order to prove (3.19a) we first observe that $\mathrm{Im}(\log(\Phi_+(\lambda + i\varepsilon)))$ takes on boundary values $\mathrm{Im}(\log(\Phi_+(\lambda + i0)))$ for a.e. $\lambda \in \mathbb{R}$ in $\mathcal{B}_1(\mathcal{H}_+)$-norm by (2.2). Next, choosing an orthonormal system $\{e_n\}_{n\in\mathbb{N}} \subset \mathcal{H}_+$, we recall that the quadratic form $(e_n, \mathrm{Im}(\log(\Phi(\lambda + i0)))e_n)_{\mathcal{H}_+}$ exists for all $\lambda \in \mathbb{R}\backslash\mathcal{E}_n$, where $\mathcal{E}_n$ has Lebesgue measure zero. Thus one observes,

$$\begin{aligned}\lim_{\varepsilon\downarrow 0}(e_m, \mathrm{Im}(\log(\Phi_+(\lambda + i\varepsilon)))e_n)_{\mathcal{H}_+} &= (e_m, \mathrm{Im}(\log(\Phi_+(\lambda + i0)))e_n)_{\mathcal{H}_+} \\ &= \pi(e_m, \Xi_+(\lambda)e_n)_{\mathcal{H}_+} \text{ for } \lambda \in \mathbb{R}\backslash\{\mathcal{E}_m \cup \mathcal{E}_n\}.\end{aligned} \tag{3.26}$$

Let $\mathcal{E} = \cup_{n\in\mathbb{N}}\mathcal{E}_n$, then $|\mathcal{E}| = 0$ ($|\cdot|$ denoting the Lebesgue measure on $\mathbb{R}$) and hence

$$\begin{aligned}&(f, \mathrm{Im}(\log(\Phi_+(\lambda + i0)))g)_{\mathcal{H}_+} = \pi(f, \Xi_+(\lambda)g)_{\mathcal{H}_+} \\ &\text{for } \lambda \in \mathbb{R}\backslash\mathcal{E} \text{ and } f, g \in \mathcal{D} = \text{lin.span}\,\{e_n \in \mathcal{H}_+ \,|\, n \in \mathbb{N}\}.\end{aligned} \tag{3.27}$$

Since $\mathcal{D}$ is dense in $\mathcal{H}_+$ and $\Xi_+(\lambda) \in \mathcal{B}(\mathcal{H}_+)$ one infers $\mathrm{Im}(\log(\Phi_+(\lambda + i0))) = \pi\Xi_+(\lambda)$ for a.e. $\lambda \in \mathbb{R}$, completing the proof. $\square$

Assuming Hypothesis 3.1 we define

$$\xi(\lambda) = \xi_+(\lambda) - \xi_-(\lambda) \text{ for a.e. } \lambda \in \mathbb{R} \tag{3.28}$$

and call $\xi(\lambda)$ (respectively, $\xi_+(\lambda)$, $\xi_-(\lambda)$) the spectral shift function associated with the pair (H_0, H) (respectively, (H_0, H_+), (H_+, H)), sometimes also denoted by $\xi(\lambda, H_0, H)$, etc., to underscore the dependence on the pair involved.

M. Krein's basic trace formula [47] is now obtained as follows.

Theorem 3.6. *Assume Hypothesis 3.1. Then* $(z \in \mathbb{C}\backslash\{\mathrm{spec}(H_0) \cup \mathrm{spec}(H)\})$

$$\mathrm{tr}_{\mathcal{H}}((H-z)^{-1} - (H_0 - z)^{-1}) = -\int_{\mathbb{R}} d\lambda\, \xi(\lambda)(\lambda - z)^{-2}. \tag{3.29}$$

Proof. Let $z \in \mathbb{C}\backslash\mathbb{R}$. By (3.22) and (3.24) we infer

$$\mathrm{tr}_{\mathcal{H}_+}(\log(\Phi_+(z))) = \int_{\mathbb{R}} d\lambda\, \xi_+(\lambda)(\lambda - z)^{-1}, \tag{3.30}$$

$$\mathrm{tr}_{\mathcal{H}_-}(\log(\widetilde{\Phi}_-(z))) = -\int_{\mathbb{R}} d\lambda\, \xi_-(\lambda)(\lambda - z)^{-1}. \tag{3.31}$$

Adding (3.13a) and (3.13b), differentiating (3.30) and (3.31) with respect to z proves (3.29) for $z \in \mathbb{C}\backslash\mathbb{R}$. The result extends to all $z \in \mathbb{C}\backslash\{\mathrm{spec}(H_0) \cup \mathrm{spec}(H)\}$ by continuity of $((H-z)^{-1} - (H_0 - z)^{-1})$ in $\mathcal{B}_1(\mathcal{H})$-norm. ☐

In particular, $\xi(\lambda)$ introduced in (3.28) is Krein's original spectral shift function. As noted in Section 2, the spectral shift operator $\Xi_+(\lambda)$ in the particular case $V = V_+$, and its relation to Krein's spectral shift function $\xi_+(\lambda)$, was first studied by Carey [15] in 1976.

Remark 3.7. (i) As shown originally by M. Krein [47], the trace formula (3.29) extends to

$$\mathrm{tr}(f(H) - f(H_0)) = \int_{\mathbb{R}} d\lambda\, \xi(\lambda) f'(\lambda) \tag{3.32}$$

for appropriate functions f. This fact has been studied by numerous authors and we refer, for instance, to [4], Ch. 19, [9]–[11], [48], [49], [58], [66], [67], [69], [70], Ch. 8 and the references therein.

(ii) Concerning scattering theory for the pair (H_0, H), we remark that $\xi(\lambda)$, for a.e. $\lambda \in \mathrm{spec}_{ac}(H_0)$ (the absolutely continuous spectrum of H_0), is related to the scattering operator at fixed energy λ by the Birman-Krein formula [8],

$$\det_{\mathcal{H}_\lambda}(S(\lambda, H_0, H)) = e^{-2\pi i \xi(\lambda)} \text{ for a.e. } \lambda \in \mathrm{spec}_{ac}(H_0). \tag{3.33}$$

Here $S(\lambda, H_0, H)$ denote the fibers in the direct integral representation of the scattering operator

$$S(H_0, H) = \int_{\mathrm{spec}_{ac}(H_0)}^{\oplus} d\lambda\, S(\lambda, H_0, H) \text{ in } \mathcal{H} = \int_{\mathrm{spec}_{ac}(H_0)}^{\oplus} d\lambda\, \mathcal{H}_\lambda$$

with respect to the absolutely continuous part $H_{0,ac}$ of H_0. This fundamental connection, originally due to Birman and Krein [8], is further discussed in [4], Ch. 19, [11], [12], [15], [42], [48], [68], [70], Ch. 8 and the literature cited therein. We briefly return to this topic in Lemma 4.7.

(iii) The standard identity ([37], Sect. IV.3)

$$\mathrm{tr}_{\mathcal{H}}((H-z)^{-1} - (H_0 - z)^{-1}) = -d\log(\det_{\mathcal{H}}(I_{\mathcal{H}} + V(H_0 - z)^{-1}))/dz \tag{3.34}$$

together with the trace formula (3.29) yields the well-known connection between perturbation determinants and $\xi(\lambda)$, also due to M. Krein [47]

$$\log(\det_{\mathcal{H}}(I_{\mathcal{H}} + V(H_0 - z)^{-1})) = \int_{\mathbb{R}} d\lambda\, \xi(\lambda)(\lambda - z)^{-1}, \tag{3.35}$$

$$\xi(\lambda) = \lim_{\varepsilon\downarrow 0} \pi^{-1}\mathrm{Im}(\log(\det_{\mathcal{H}}(I_{\mathcal{H}} + V(H_0 - (\lambda + i0))^{-1}))) \text{ for a.e. } \lambda \in \mathbb{R}, \tag{3.36}$$

$$\mathrm{tr}_{\mathcal{H}}(V) = \int_{\mathbb{R}} d\lambda\, \xi(\lambda), \qquad \int_{\mathbb{R}} d\lambda\, |\xi(\lambda)| \leq ||V||_1. \tag{3.37}$$

This is discussed in more detail, for instance, in [4], Ch. 19, [11], [15], [46], [48], [50], [66]–[68], [70]. Relation (3.36) and the analog of (2.2) for $d(AE_H(\lambda)B)/d\lambda$, where $H = H_0 + V$, $V = B^*A$, $A, B \in \mathcal{B}_2(\mathcal{H})$, $V = V^*$, leads to the expression

$$\xi(\lambda) = (-2\pi i)^{-1}\,\mathrm{tr}_{\mathcal{H}}(\log(I_{\mathcal{H}} - 2\pi i(I_{\mathcal{H}} - A(H - \lambda - i0)^{-1}B^*)(d(AE_H(\lambda)B^*)/d\lambda)))$$

for a.e. $\lambda \in \mathbb{R}$ (cf., e.g., [4], Sects. 3.4.4 and 19.1.4).

For numerous additional properties and applications of Krein's spectral shift function we refer to citeEP97, [25], [40], [42], [43], [59], [68] and the references therein.

4. Some Applications

In this section we consider some applications of the formalism developed in Sections 2 and 3.

We start by recalling the simple proof of spectral averaging and its relation to Krein's spectral shift function in [33], a circle of ideas originating with Birman and Solomyak [10].

For this purpose we assume the following.

Hypothesis 4.1. *Let H_0 be a self-adjoint operator in $\mathcal{H}$ with* $\mathrm{dom}(H_0)$*, and assume $\{V(s)\}_{s\in\Omega} \subset \mathcal{B}_1(\mathcal{H})$ to be a family of self-adjoint trace class operators in $\mathcal{H}$, where $\Omega \subseteq \mathbb{R}$ denotes an open interval. Moreover, suppose that $V(s)$ is continuously differentiable with respect to $s \in \Omega$ in trace norm.*

To begin our discussions we temporarily assume that $V(s) \geq 0$, that is, we suppose

$$V(s) = K(s)K(s)^*, \quad s \in \Omega \tag{4.1}$$

for some $K(s) \in \mathcal{B}_2(\mathcal{H})$, $s \in \Omega$. Given Hypothesis 4.1 we define the self-adjoint operator $H(s)$ in $\mathcal{H}$ by

$$H(s) = H_0 + V(s), \quad \mathrm{dom}(H(s)) = \mathrm{dom}(H_0), \quad s \in \Omega. \tag{4.2}$$

In analogy to (3.5) and (3.6) we introduce in $\mathcal{H}$ ($s \in \Omega$, $z \in \mathbb{C}\backslash\mathbb{R}$),

$$\Phi(z, s) = I_{\mathcal{H}} + K(s)^*(H_0 - z)^{-1}K(s) \tag{4.3}$$

and hence infer from Lemma 3.2 that

$$\Phi(z, s)^{-1} = I_{\mathcal{H}} - K(s)^*(H(s) - z)^{-1}K(s). \tag{4.4}$$

The following is an elementary but useful result needed in the context of Theorem 4.3.

Lemma 4.2. *Assume Hypothesis 4.1 and* (4.1). *Then* ($s \in \Omega$, $z \in \mathbb{C}\backslash\mathbb{R}$),

$$d\,\mathrm{tr}_{\mathcal{H}}(\log(\Phi(z,s)))/ds = \mathrm{tr}_{\mathcal{H}}(V'(s)(H(s)-z)^{-1}). \tag{4.5}$$

Next, applying Lemma 3.5 to $\Phi(z,s)$ in (4.3) one infers ($s \in \Omega$),

$$\log(\Phi(z,s)) = \int d\lambda\, \Xi(\lambda,s)(\lambda - z)^{-1}, \tag{4.6}$$

$$0 \le \Xi(\lambda,s) \le I_{\mathcal{H}}, \quad \Xi(\lambda,s) \in \mathcal{B}_1(\mathcal{H}) \text{ for a.e. } \lambda \in \mathbb{R}, \tag{4.7}$$
$$||\Xi(\cdot,s)||_1 \in L^1(\mathbb{R}; d\lambda),$$

where $\Xi(\lambda,s)$ is associated with the pair $(H_0, H(s))$, assuming $H(s) \ge H_0$, $s \in \Omega$.

The principal result on averaging the spectral measure of $\{E_{H(s)}(\lambda)\}_{\lambda\in\mathbb{R}}$ of $H(s)$ as proven in [33] then reads as follows.

Theorem 4.3. ([33].) *Assume Hypothesis 4.1 and* $[s_1, s_2] \subset \Omega$. *Let* $\xi(\lambda,s)$ *be the spectral shift function associated with the pair* $(H_0, H(s))$ (*cf.* (3.28)), *where* $H(s)$ *is defined by* (4.2) (*and we no longer suppose* $H(s) \ge H_0$). *Then*

$$\int_{s1}^{s_2} ds\,(d(\mathrm{tr}_{\mathcal{H}}(V'(s)E_{H(s)}(\lambda)))) = (\xi(\lambda,s_2) - \xi(\lambda,s_1))d\lambda. \tag{4.8}$$

Remark 4.4. (i) In the special case of averaging over the boundary condition parameter for half-line Sturm-Liouville operators (effectively a rank-one resolvent perturbation problem), Theorem 4.3 has first been derived by Javrjan [38], [39]. The case of rank-one perturbations was recently treated in detail by Simon [64]. The general case of trace class perturbations is due to Birman and Solomyak [10] using an approach of Stieltjes' double operator integrals. Birman and Solomyak treat the case $V(s) = sV$, $V \in \mathcal{B}_1(\mathcal{H})$, $s \in [0,1]$. A short proof of (4.8) (assuming $V'(s) \ge 0$) has recently been given by Simon [65].
(ii) We note that variants of (4.8) in the context of one-dimensional Sturm-Liouville operators (i.e., variants of Javrjan's results in [38], [39]) have been repeatedly rediscovered by several authors. In particular, the absolute continuity of averaged spectral measures (with respect to boundary condition parameters or coupling constants of rank-one perturbations) has been used to prove localization properties of one-dimensional random Schrödinger operators (see, e.g., [14], [17], [18], [19], Ch. VIII, [20], [21], [43]–[45], [57], Ch. V, [63], [64]).
(iii) We emphasize that Theorem 4.3 applies to unbounded operators (and hence to random Schrödinger operators bounded from below) as long as appropriate relative trace class conditions (either with respect to resolvent or semigroup perturbations) are satisfied.
(iv) In the special case $V'(s) \ge 0$, the measure

$$d(\mathrm{tr}_{\mathcal{H}}(V'(s)E_{H(s)}(\lambda))) = d(\mathrm{tr}_{\mathcal{H}}(V'(s)^{1/2}E_{H(s)}(\lambda)V'(s)^{1/2}))$$

in (4.8) represents a positive measure.

In the special case of a sign-definite perturbation of H_0 of the form sKK^*, one can in fact prove an operator-valued averaging formula as follows.

Theorem 4.5. ([33].) *Assume Hypothesis 3.1 and* $J = I_{\mathcal{H}}$. *Then*

$$\int_0^1 ds\, d(K^* E_{H_0+sKK^*}(\lambda)K) = \Xi(\lambda)d\lambda, \tag{4.9}$$

where $\Xi(\cdot)$ *is the spectral shift operator associated with*

$$\Phi(z) = I_{\mathcal{H}} + K^*(H_0 - z)^{-1}K, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{4.10}$$

that is,

$$\log(\Phi(z)) = \int_{\mathbb{R}} d\lambda\, \Xi(\lambda)(\lambda - z)^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{4.11}$$

$$0 \leq \Xi(\lambda) \in \mathcal{B}_1(\mathcal{H}) \text{ for a.e. } \lambda \in \mathbb{R}, \quad \|\Xi(\cdot)\|_1 \in L^1(\mathbb{R}; d\lambda). \tag{4.12}$$

Proof. An explicit computation shows

$$\begin{aligned}
&(\lambda - \Phi(z))^{-1} = -(1-\lambda)^{-1} \\
&\quad \times (I_{\mathcal{H}} - (1-\lambda)^{-1}K^*(H_0 + (1-\lambda)^{-1}KK^* - z)^{-1}K) \in \mathcal{B}(\mathcal{H})
\end{aligned} \tag{4.13}$$

for all $\lambda < 0$. Since $\log(\Phi(z)) = \ln(\Phi(z))$ for $z \in \mathbb{C}_+$ as a result of analytic continuation, one obtains

$$\begin{aligned}
\log(\Phi(z)) &= \int_{\mathbb{R}} d\lambda\, \Xi(\lambda)(\lambda - z)^{-1} \\
= \ln(\Phi(z)) &= \int_{-\infty}^{0} d\lambda\, ((\lambda - \Phi(z))^{-1} - \lambda(1+\lambda^2)^{-1}I_{\mathcal{H}}) \\
&= \int_{-\infty}^{0} d\lambda\, (1-\lambda)^{-2}K^*(H_0 + (1-\lambda)^{-1}KK^* - z)^{-1}K \\
&= \int_0^1 ds \int_{\mathbb{R}} d(K^*E_{H_0+sKK^*}(\lambda)K)(\lambda - z)^{-1} \\
&= \int_{\mathbb{R}} (\lambda - z)^{-1} \int_0^1 ds\, d(K^*E_{H_0+sKK^*}(\lambda)K)
\end{aligned} \tag{4.14}$$

proving (4.9). (Here the interchange of the λ and s integrals follows from Fubini's theorem considering (4.14) in the weak sense.) □

As a consequence of Theorem 4.5 one obtains

$$\int_{s_1}^{s_2} ds\, d(K^*E_{H_0+sKK^*}(\lambda)K) = \Xi(\lambda, s_2) - \Xi(\lambda, s_1), \tag{4.15}$$

where $\Xi(\lambda, s)$ is the spectral shift operator associated with $\Phi(z, s) = I_{\mathcal{H}} + sK^*(H_0 - z)^{-1}K$, $s \in [s_1, s_2]$. This yields an alternative proof of the following result of Carey [15].

Lemma 4.6. ([15].) *Assume Hypothesis 3.1 and* $J = I_{\mathcal{H}}$. *Then*

$$K^*K = \int_{\mathbb{R}} d\lambda\, \Xi(\lambda), \tag{4.16}$$

with $\Xi(\lambda)$ *given by* (4.11).

Proof. Given $f \in \mathcal{H}$ one infers

$$\begin{aligned}
\left(\int_{\mathbb{R}} \int_0^1 ds\, d(K^*E_{H_0+sKK^*}(\lambda)K)f, f \right) &= \int_0^1 ds \int_{\mathbb{R}} d(K^*E_{H_0+sKK^*}(\lambda)Kf, f) \\
&= \int_0^1 ds ||Kf||^2 = ||Kf||^2
\end{aligned} \tag{4.17}$$

by Fubini's theorem. Combining (4.9) and (4.17) one concludes

$$||Kf||^2 = \Big(\int_{\mathbb{R}} d\lambda\, \Xi(\lambda) f, f \Big). \tag{4.18}$$

Since K^*K and $\int_{\mathbb{R}} d\lambda\, \Xi(\lambda)$ are both bounded operators and by (4.18) their quadratic forms coincide, one obtains (4.16). ☐

For nonnegative perturbations $V \geq 0$, $V \in \mathcal{B}_1(\mathcal{H})$, the particular choice $K = K^* = V^{1/2}$ then reconstructs V via

$$V = \int_{\mathbb{R}} d\lambda\, \Xi(\lambda) \tag{4.19}$$

as a consequence of Lemma 4.6.

The case of nonpositive perturbations can be treated in an analogous way. The general case of sign indefinite perturbations will be considered elsewhere [32].

Next, combining some results of Kato [42] and Carey [15], we briefly turn to scattering theory for the pair (H_0, H), $H = H_0 + KK^*$, assuming Hypothesis 3.1 and $J = I_{\mathcal{H}}$. We pick an interval $(a,b) \subseteq \mathbb{R}$ and assume that H_0 is spectrally absolutely continuous on (a,b), that is, $E_{H_0}(\lambda) = E_{H_0,\text{a.c.}}(\lambda)$, $\lambda \in (a,b)$, where $\{E_{H_0}(\lambda)\}_{\lambda\in\mathbb{R}}$ denotes the family of orthogonal spectral projections of H_0. As discussed in connection with Theorem 2.2,

$$\Phi(\lambda \pm i0) = \lim_{\varepsilon\downarrow 0} \Phi(\lambda \pm i\varepsilon), \tag{4.20}$$

exist for a.e. $\lambda \in \mathbb{R}$ in $\mathcal{B}_2(\mathcal{H})$-norm (actually in $\mathcal{B}_p(\mathcal{H})$-norm for all $p > 1$) and

$$A(\lambda) = d(K^* E_{H_0}(\lambda) K)/d\lambda \in \mathcal{B}_1(\mathcal{H}), \tag{4.21}$$

$$\lim_{\varepsilon\downarrow 0} \pi^{-1} \text{Im}(\Phi(\lambda + i\varepsilon)) = A(\lambda) \text{ for a.e. } \lambda \in \mathbb{R} \tag{4.22}$$

in $\mathcal{B}_1(\mathcal{H})$-norm (cf., e.g., [4], Sect. 3.4.4), with $\Phi(z)$ defined as in (4.10). Following Kato [42], one considers $\text{ran}(K) = K\mathcal{H}$ and defines the semi-inner product $(\cdot,\cdot)_{\text{ran}(K),\lambda}$, $\lambda \in (a,b)$, by

$$(x,y)_{\text{ran}(K),\lambda} = (f, A(\lambda) g)_{\mathcal{H}} \text{ for a.e. } \lambda \in (a,b),\ x = Kf,\ y = Kg,\ f,g \in \mathcal{H}. \tag{4.23}$$

Denoting by $\mathcal{K}(\lambda) = \overline{(\text{ran}(K); (\cdot,\cdot)_{\text{ran}(K),\lambda})}$, the completion of $\text{ran}(K)$ with respect to $(\cdot,\cdot)_{\text{ran}(K),\lambda}$, the fibers $S(\lambda, H_0, H)$, $\lambda \in (a,b)$ in the direct integral representation of the (local) scattering operator $S(H_0,H)P_{H_0}((a,b))$ ($P_{H_0}((a,b))$ the corresponding orthogonal spectral projection of H_0 associated with the interval (a,b)) then can be identified with the unitary operator

$$(I_{\mathcal{K}(\lambda)} + KK^*(H_0 - \lambda - i0)^{-1})^{-1}(I_{\mathcal{K}(\lambda)} + KK^*(H_0 - \lambda + i0)^{-1}) \text{ for a.e. } \lambda \in (a,b) \tag{4.24}$$

on $\mathcal{K}(\lambda)$. Introducing $\mathcal{H}(\lambda) = \overline{(\mathcal{H}; (\cdot,\cdot)_\lambda)}$, the completion of $\mathcal{H}$ with respect to the semi-inner product

$$(f,g)_\lambda = (f, A(\lambda) g)_{\mathcal{H}} \text{ for a.e. } \lambda \in (a,b), \tag{4.25}$$

the isometric isomorphism between $\mathcal{K}(\lambda)$ and $\mathcal{H}(\lambda)$, $\lambda \in (a,b)$ then yields that (4.24) is unitarily equivalent to (cf. [42]),

$$S(\lambda) = \Phi(\lambda + i0)^{-1} \Phi(\lambda - i0) \text{ for a.e. } \lambda \in (a,b). \tag{4.26}$$

Arguing as in section 5 of Carey [15], Asano's result [3] on strong boundary values for vector-valued singular integrals of Cauchy-type then yields the following connection between $S(\lambda)$ in (4.26) and $\Xi(\lambda)$, $\lambda \in (a,b)$ in (4.11).

Lemma 4.7. *Assume Hypothesis 3.1 with $J = I_{\mathcal{H}}$ and suppose H_0 is spectrally absolutely continuous on $(a,b) \subseteq \mathbb{R}$. Then $S(\lambda)$ given by (4.26) satisfies*

$$\begin{aligned} S(\lambda) &= \exp\bigg(- P.V. \int_{\mathbb{R}} d\mu \, \Xi(\mu)(\mu-\lambda)^{-1} - i\pi\Xi(\lambda)\bigg) \times \\ &\times \exp\bigg(P.V. \int_{\mathbb{R}} d\mu \, \Xi(\mu)(\mu-\lambda)^{-1} - i\pi\Xi(\lambda)\bigg) \text{ for a.e. } \lambda \in (a,b), \end{aligned} \tag{4.27}$$

where $P.V. \int_{\mathbb{R}} d\mu \,\cdot$ denotes the principal value. This implies the Birman-Krein formula

$$det_{\mathcal{H}(\lambda)}(S(\lambda)) = e^{-2\pi i \xi(\lambda)} \text{ for a.e. } \lambda \in (a,b), \tag{4.28}$$

with $\xi(\lambda) = \mathrm{tr}_{\mathcal{H}}(\Xi(\lambda))$.

Proof. Asano's result [3], applied to the Hilbert space of $\mathcal{B}_2(\mathcal{H})$-operators yields

$$\begin{aligned} &\operatorname*{s-lim}_{\varepsilon\downarrow 0} \int_{\mathbb{R}} d\mu \, \Xi(\mu)(\mu-(\lambda \pm i\varepsilon))^{-1} \\ &= \mathrm{P.V.} \int_{\mathbb{R}} d\mu \, \Xi(\mu)(\mu-\lambda)^{-1} \pm i\pi\Xi(\lambda) \in \mathcal{B}_2(\mathcal{H}) \text{ for a.e. } \lambda \in \mathbb{R} \end{aligned} \tag{4.29}$$

(with s-lim denoting convergence in $\mathcal{B}_2(\mathcal{H})$-norm). Combining (4.29) (4.26), and (4.11) then yields (4.27). ☐

It should be noted that (4.26) is not necessarily the usually employed scattering operator at fixed energy $\lambda \in (a,b)$. In concrete applications one infers that $0 \leq A(\lambda) \in \mathcal{B}_1(\mathcal{H})$ typically factors into a product

$$A(\lambda) = B(\lambda)^* B(\lambda), \quad B(\lambda) \in \mathcal{B}_2(\mathcal{H}, \mathcal{L}), \tag{4.30}$$

with $\mathcal{L}$ another Hilbert space (e.g., $\mathcal{L} = L^2(S^{n-1})$ in connection with potential scattering in $\mathbb{R}^n$, $n \geq 2$ and $\mathcal{L} = \mathbb{C}^2$ for $n = 1$) and hence usually $S(\lambda)$ in (4.26) is then repaced by the unitary operator

$$\widetilde{S}(\lambda) = I_{\mathcal{L}} - 2\pi i B(\lambda)(I_{\mathcal{H}} + \Phi(\lambda + i0))^{-1} B(\lambda)^* \text{ for a.e. } \lambda \in (a,b) \tag{4.31}$$

in $\mathcal{L}$.

For brevity we only considered positive perturbations $V = KK^*$. The general case of perturbations of the type $V = KJK^*$ will be considered elsewhere [32].

Next, assume Hypothesis 3.1 and $J = I_{\mathcal{H}}$, introduce

$$V = KK^*, \tag{4.32}$$

and define the family of self-adjoint operators

$$H(s) = H_0 + sV, \quad s \in \mathbb{R}. \tag{4.33}$$

In accordance with (3.5)–(3.7) introduce the following bounded operators

$$\Phi_+(z,s) = I_{\mathcal{H}} + sK^*(H_0 - z)^{-1}K, \quad s > 0, \tag{4.34}$$

$$\widetilde{\Phi}_-(z,s) = I_{\mathcal{H}} + sK^*(H_+ - z)^{-1}K, \quad s < 0, \tag{4.35}$$

for $z \in \mathbb{C} \backslash \mathbb{R}$.

By Lemma 3.5 we have the representations

$$\log(\Phi_+(z,s)) = \int_{\mathbb{R}} d\lambda\, \Xi_+(\lambda,s)(\lambda-z)^{-1}, \quad s>0 \tag{4.36}$$

$$\log(\widetilde{\Phi}_-(z,s)) = -\int_{\mathbb{R}} d\lambda\, \Xi_-(\lambda,s)(\lambda-z)^{-1}, \quad s<0, \tag{4.37}$$

where $\Xi_+(\lambda,s)$ (respectively, $\Xi_-(\lambda,s)$) is the spectral shift operator associated with the pair $(H_0, H(s))$ for $s>0$ (respectively, for $s<0$).

Moreover, by (3.19a) and (3.19b) we have

$$\Xi_+(\lambda,s) = \lim_{\varepsilon\downarrow 0} \pi^{-1}\mathrm{Im}(\log(\Phi_+(\lambda+i\varepsilon,s))), \quad s>0, \tag{4.38}$$

$$\Xi_-(\lambda,s) = -\lim_{\varepsilon\downarrow 0} \pi^{-1}\mathrm{Im}(\log(\widetilde{\Phi}_-(\lambda+i\varepsilon,s))), \quad s<0. \tag{4.39}$$

Theorem 4.8. *Assume Hypothesis 3.1 and $J=I_{\mathcal{H}}$. Set $V=KK^*\geq 0$, suppose that $\mathcal{P}=\mathrm{ran}(V)$ is a finite-dimensional subspace of $\mathcal{H}$, and denote by P the orthogonal projection onto $\mathcal{P}$. In addition, let*

$$T(z) = V^{1/2}(H_0-z)^{-1}V^{1/2}, \quad z\in\mathbb{C}_+. \tag{4.40}$$

Then the boundary values

$$T(\lambda) = \text{n-}\lim_{\varepsilon\downarrow 0} T(\lambda+i\varepsilon) \tag{4.41}$$

exist for a.e. $\lambda\in\mathbb{R}$. For such $\lambda\in\mathbb{R}$, $T(\lambda)$ is reduced by the subspace $\mathcal{P}$ and the part $T(\lambda)|_{\mathcal{P}}$ of the operator $T(\lambda)$ restricted to the subspace $\mathcal{P}$ is invertible for a. e. $\lambda\in\mathbb{R}$. The corresponding set of $\lambda\in\mathbb{R}$ such that $T(\lambda)|_{\mathcal{P}}$ is invertible in $\mathcal{P}=P\mathcal{H}$ is denoted by Λ. Finally, for all $\lambda\in\Lambda$ one obtains the following asymptotic expansion

$$\Xi_+(\lambda,s)+\Xi_-(\lambda,-s) \underset{s\uparrow\infty}{=} P - 2(\pi s)^{-1} P\,\mathrm{Im}(T(\lambda)|_{\mathcal{P}})^{-1}P + O(s^{-2})P. \tag{4.42}$$

Proof. The a.e. existence of the norm limit in (4.41) and the invertibility of $T(\lambda)|_{\mathcal{P}}$ in $\mathcal{P}=P\mathcal{H}$ is a consequence of Lemma 2.4. By definition (2.11) of logarithms of dissipative operators one infers

$$\log(\Phi_+(\lambda+i\varepsilon,s)) = -i\int_0^\infty dt\big((sT(\lambda+i\varepsilon)+(1+it)I_{\mathcal{H}})^{-1} - (1+it)^{-1}I_{\mathcal{H}}\big), \quad s>0,\ \varepsilon>0. \tag{4.43}$$

By (4.40), $\log(\Phi_+(\lambda+i\varepsilon,s))$ is reduced by the subspace $\mathcal{P}=P\mathcal{H}$ and

$$\log(\Phi_+(\lambda+i\varepsilon,s))|_{\mathcal{H}\ominus\mathcal{P}} = 0. \tag{4.44}$$

The operator $\log(\Phi_+(\lambda+i\varepsilon,s))|_{\mathcal{P}}$ restricted to the invariant subspace $\mathcal{P}$ then can be represented as follows

$$\begin{aligned}&\log(\Phi_+(\lambda+i\varepsilon,s))|_{\mathcal{P}}\\ &= -i\int_0^\infty dt\big((sT(\lambda+i\varepsilon)|_{\mathcal{P}}+(1+it)I_{\mathcal{P}})^{-1} - (1+it)^{-1}I_{\mathcal{P}}\big),\\ &\qquad s>0,\ \varepsilon>0.\end{aligned} \tag{4.45}$$

For $\lambda\in\Lambda$, the operator $(I+sT(\lambda))|_{\mathcal{P}}$ is invertible for $s>0$ sufficiently large and therefore, for such $s>0$ one can go to the limit $\varepsilon\to 0$ in (4.45) to arrive at

$$\log(\Phi_+(\lambda+i0,s))|_{\mathcal{P}}$$

$$= -i\int_0^\infty dt\big((sT(\lambda)|_{\mathcal P} + (1+it)I_{\mathcal P})^{-1} - (1+it)^{-1}I_{\mathcal P}\big),\tag{4.46}$$
$$s>0 \text{ sufficiently large}, \ \lambda\in\Lambda.$$

Since for $s<0$ the operator $-\widetilde{\Phi}_-(\lambda+i\varepsilon,s)$ is dissipative, one concludes as in (2.20) that

$$\begin{aligned}\log(\widetilde{\Phi}_-(\lambda+i\varepsilon,s)) &= \big(\log(\widetilde{\Phi}_-^*(\lambda+i\varepsilon,s))\big)^*\\ &= i\int_0^\infty dt\big((sT(\lambda+i\varepsilon)+(1-it)I_{\mathcal H})^{-1} - (1-it)^{-1}I_{\mathcal H}\big)\\ &= -i\int_0^\infty dt\big((|s|T(\lambda+i\varepsilon)+(it-1)I_{\mathcal H})^{-1} + (1-it)^{-1}I_{\mathcal H}\big),\end{aligned}\tag{4.47}$$
$$s<0,\ \varepsilon>0.$$

Similarly one concludes that $\log(\widetilde{\Phi}_-(\lambda+i0,s))$, $\lambda\in\Lambda$ is reduced by the subspace $\mathcal P$ and

$$\begin{aligned}&\log(\widetilde{\Phi}_-(\lambda+i0,s))|_{\mathcal P}\\ &= -i\int_0^\infty dt\big((sT(\lambda)|_{\mathcal P} + (it-1)I_{\mathcal P})^{-1} - (1+it)^{-1}I_{\mathcal P}\big),\end{aligned}\tag{4.48}$$
$$s>0 \text{ sufficiently large}, \ \lambda\in\Lambda.$$

By (4.38) and (4.39) one obtains for $s>0$

$$\Xi_+(\lambda,s)+\Xi_-(\lambda,-s) = \pi^{-1}\mathrm{Im}\big(\log(\Phi_+(\lambda+i0,s)) - \log(\widetilde{\Phi}_-(\lambda+i0,s))\big),\tag{4.49}$$
$$\lambda\in\Lambda.$$

Combining (4.46) and (4.48) and taking into account the fact that

$$\log(\Phi_+(\lambda+i0,s))|_{\mathcal H\ominus\mathcal P} = \log(\widetilde{\Phi}_-(\lambda+i0,s))|_{\mathcal H\ominus\mathcal P} = 0, \quad \lambda\in\Lambda,\tag{4.50}$$

one concludes that the subspace $\mathcal P$ reduces $\Xi_+(\lambda,s)+\Xi_-(\lambda,-s)$ and that

$$\big(\Xi_+(\lambda,s)+\Xi_-(\lambda,-s)\big)|_{\mathcal H\ominus\mathcal P} = 0, \quad \lambda\in\Lambda.\tag{4.51}$$

Moreover, for $\lambda\in\Lambda$,

$$\begin{aligned}&\big(\Xi_+(\lambda,s)+\Xi_-(\lambda,-s)\big)|_{\mathcal P}\\ &= \pi^{-1}\mathrm{Im}\bigg(-i\int_0^\infty dt\big((sT(\lambda)|_{\mathcal P}+(1+it)I_{\mathcal P})^{-1} - (sT(\lambda)|_{\mathcal P}+(it-1)I_{\mathcal P})^{-1}\bigg)\\ &+ \pi^{-1}\mathrm{Im}\bigg(i\int_0^\infty dt\big(((1+it)^{-1}+(1-it)^{-1})I_{\mathcal P}\bigg)\\ &= \pi^{-1}\mathrm{Im}\bigg(2i\int_0^\infty dt\big((sT(\lambda)|_{\mathcal P}+(it+1)I_{\mathcal P})^{-1}(sT(\lambda)|_{\mathcal P}+(it-1)I_{\mathcal P})^{-1}\big)\bigg) + I|_{\mathcal P}.\end{aligned}\tag{4.52}$$

Changing variables $t\to s^{-1}t$ using the fact that $T(\lambda)|_{\mathcal P}$ is invertible for $\lambda\in\Lambda$ then yields

$$\int_0^\infty dt\big((sT(\lambda)|_{\mathcal P}+(it+1)I_{\mathcal P})^{-1}(sT(\lambda)|_{\mathcal P}+(it-1)I_{\mathcal P})^{-1}\big)$$

$$
\begin{aligned}
&= s^{-1}\int_0^\infty dt\big((T(\lambda)|_{\mathcal{P}} + (it+s^{-1})I_{\mathcal{P}})^{-1}(T(\lambda)|_{\mathcal{P}} + (it-s^{-1})I_{\mathcal{P}})^{-1}\big)\\
&\underset{s\uparrow\infty}{=} s^{-1}\int_0^\infty dt\big((T(\lambda)|_{\mathcal{P}} + itI_{\mathcal{P}})^{-2} + O(s^{-2})P\\
&\underset{s\uparrow\infty}{=} s^{-1}i((T(\lambda)|_{\mathcal{P}})^{-1} + O(s^{-2})P, \qquad (4.53)
\end{aligned}
$$

where in obvious notation $O(s^{-2})$ denotes a bounded operator in $\mathcal{P}$ whose norm is of order $O(s^{-2})$ as $s\uparrow\infty$. Combining (4.52) and (4.53) we get the asymptotic representation

$$
\big(\Xi_+(\lambda,s)+\Xi_-(\lambda,-s)\big)|_{\mathcal{P}} \underset{s\uparrow\infty}{=} I|_{\mathcal{P}} - 2(\pi s)^{-1}\mathrm{Im}\big((T(\lambda)|_{\mathcal{P}})^{-1}\big) + O(s^{-2})P, \quad \lambda\in\Lambda. \tag{4.54}
$$

Together with (4.51) this proves (4.42). □

Taking the trace of (4.42) and going to the limit $s\uparrow\infty$, Theorem 4.8 implies the following result first proved by Simon (see [65]) for finite-rank nonnegative perturbations V,

$$
\lim_{s\uparrow\infty}(\xi(\lambda,H_0,H_0+sV)-\xi(\lambda,H_0,H_0-sV)) = \mathrm{rank}(V), \quad \lambda\in\Lambda, \tag{4.55}
$$

where

$$
\xi(\lambda,H_0,H_0+sV) = \mathrm{tr}(\Xi_+(\lambda,s)), \quad s>0 \tag{4.56}
$$

and

$$
\xi(\lambda,H_0,H_0-sV) = -\,\mathrm{tr}(\Xi_-(\lambda,s)), \quad s>0 \tag{4.57}
$$

are spectral shift functions associated with the pairs $(H_0,H+sV)$, and $(H_0,H-sV)$, $s>0$, respectively.

Finally we turn to an application concerning an approach to abstract trace formulas based on perturbation theory for pairs of self-adjoint extensions of a common closed, symmetric, densely defined linear operator $\dot H$ in some complex separable Hilbert space $\mathcal{H}$. We first treat the simplest case of deficiency indices $(1,1)$ and hint at extensions to the case of deficiency indices (n,n), $n\in\mathbb{N}$ at the end. These results are applicable to one-dimensional (matrix-valued) Schrödinger operators.

We start by setting up the basic formalism. Assuming

$$
\mathrm{def}\,(\dot H) = (1,1), \tag{4.58}
$$

we use von Neumann's parametrization of all self-adjoint extensions H_α, $\alpha\in[0,\pi)$, in the usual form

$$
\begin{aligned}
&H_\alpha(f+c(u_+ + e^{2i\alpha}u_-)) = \dot Hf + c(iu_+ - ie^{2i\alpha}u_-), \quad \alpha\in[0,\pi),\\
&\mathrm{dom}(H_\alpha) = \{f + c(iu_+ - ie^{2i\alpha}u_-)\in\mathrm{dom}(\dot H^*)\,|\, f\in\mathrm{dom}(\dot H),\, c\in\mathbb{C}\}, \qquad (4.59)
\end{aligned}
$$

where

$$
u_\pm\in\mathrm{dom}(\dot H^*), \quad \dot H^*u_\pm = \pm iu_\pm, \quad \|u_\pm\|_{\mathcal{H}} = 1. \tag{4.60}
$$

Introducing the Donoghue m-function (cf. [23], [31], [34], [36]) associated with the pair $(\dot H, H_\alpha)$ by

$$
m_\alpha(z) = z + (1+z^2)(u_+,(H_\alpha - z)^{-1}u_+)_{\mathcal{H}}, \quad z\in\mathbb{C}\backslash\mathbb{R},\ \alpha\in[0,\pi), \tag{4.61}
$$

one verifies

$$m_\beta(z) = \frac{-\sin(\beta-\alpha)+\cos(\beta-\alpha)m_\alpha(z)}{\cos(\beta-\alpha)+\sin(\beta-\alpha)m_\alpha(z)}, \quad \alpha,\beta\in[0,\pi), \tag{4.62}$$

and obtains Krein's formula for the resolvent difference of two self-adjoint extensions H_α, H_β of $\dot H$ (cf., [1], Sect. 84, [34]),

$$\begin{aligned}(H_\alpha-z)^{-1}-(H_\beta-z)^{-1} = (m_\alpha(z)+\cot(\beta-\alpha))^{-1}(u_+(\overline{z}),\cdot)_{\mathcal H}u_+(z),&\\ z\in\mathbb{C}\backslash\mathbb{R},\ \alpha,\beta\in[0,\pi),&\end{aligned} \tag{4.63}$$

where

$$u_+(z) = (H_\alpha-i)(H_\alpha-z)^{-1}, \quad z\in\mathbb{C}\backslash\mathbb{R}. \tag{4.64}$$

For later reference we note the useful facts,

$$(u_+(\overline{z}_1),u_+(z_2))_{\mathcal H} = \frac{m_\alpha(z_1)-m_\alpha(z_2)}{z_1-z_2}, \quad z_1,z_2\in\mathbb{C}\backslash\mathbb{R}, \tag{4.65}$$

$$(u_+(\overline{z}),u_+(z))_{\mathcal H} = \frac{d}{dz}m_\alpha(z), \quad z\in\mathbb{C}\backslash\mathbb{R}. \tag{4.66}$$

Next, we consider a bounded self-adjoint operator V in $\mathcal H$,

$$V=V^*\in\mathcal{B}(\mathcal H) \tag{4.67}$$

and introduce an "unperturbed" operator $\dot H^{(0)} = \dot H - V$ in $\mathcal H$ such that

$$\dot H = \dot H^{(0)}+V, \quad \mathrm{dom}(\dot H) = \mathrm{dom}(\dot H^{(0)}). \tag{4.68}$$

Consequently,

$$\dot H^* = \dot H^{(0)*}+V, \quad \mathrm{dom}(\dot H^*) = \mathrm{dom}(\dot H^{(0)*}). \tag{4.69}$$

In addition, we pick $\alpha,\alpha^{(0)}\in[0,\pi)$ such that

$$\mathrm{dom}(H_\alpha) = \mathrm{dom}(H^{(0)}_{\alpha^{(0)}}). \tag{4.70}$$

Formulas (4.58)–(4.66) then apply to the self-adjoint extensions of $\dot H^{(0)}$ and in obvious notation we denote corresponding quantities associated with $\dot H^{(0)}$ by $\dot H^{(0)*}$, $H^{(0)}_{\alpha^{(0)}}$, $u^{(0)}_\pm$, $u^{(0)}_+(z)$, $m^{(0)}_{\alpha^{(0)}}(z)$, $\alpha^{(0)}\in[0,\pi)$, etc. A fundamental link between $\dot H^{(0)*}$ and $\dot H^*$ is provided by the following result.

Lemma 4.9. *Assume* (4.67) *and* (4.68) *and let* $z\in\mathbb{C}\backslash\mathbb{R}$. *Then* $(I_{\mathcal H}-(H_\alpha-z)^{-1}V)$, *is invertible,*

$$(I_{\mathcal H}-(H_\alpha-z)^{-1}V)^{-1} = (I_{\mathcal H}+(H^{(0)}_{\alpha^{(0)}}-z)^{-1}V) \tag{4.71}$$

and

$$\ker(\dot H^*-zI_{\mathcal H}) = (I_{\mathcal H}-(H_\alpha-z)^{-1}V)\ker(\dot H^{(0)*}-zI_{\mathcal H}). \tag{4.72}$$

In particular,

$$u_+(z) = c(I_{\mathcal H}-(H_\alpha-z)^{-1}V)u^{(0)}_+(z), \tag{4.73}$$

where $c>0$ *is determined by the requirement* $\|u_+(i)\|_{\mathcal H}=1$.

Proof. Equation (4.71) is clear from the identities

$$\begin{aligned} I_{\mathcal{H}} &= (I_{\mathcal{H}} - (H_\alpha - z)^{-1}V)(I_{\mathcal{H}} + (H_\alpha^{(0)} - z)^{-1}V) \\ &= (I_{\mathcal{H}} + (H_\alpha^{(0)} - z)^{-1}V)(I_{\mathcal{H}} - (H_\alpha - z)^{-1}V) \end{aligned} \tag{4.74}$$

and (4.62) follows since $(H_\alpha - z)^{-1}$ maps $\mathcal{H}$ into $\mathrm{dom}(\dot{H}^*) = \mathrm{dom}(\dot{H}^{(0)*})$ and hence

$$\begin{aligned} &(\dot{H}^* - z)(I_{\mathcal{H}} - (H_\alpha - z)^{-1}V)g = (\dot{H}^* - z)g - Vg \\ &= (\dot{H}^{(0)*} + V - z)g - Vg = (\dot{H}^{(0)*} - z)g = 0, \quad g \in \ker(\dot{H}^{(0)*} - zI_{\mathcal{H}}). \end{aligned} \tag{4.75}$$

Equation (4.73) is then clear from (4.71), (4.72). □

In the following we assume in addition that $\dot{H}^{(0)}$ is bounded from below, that is,

$$\dot{H}^{(0)} \geq CI_{\mathcal{H}} \text{ for some } C \in \mathbb{R} \tag{4.76}$$

and choose $\beta, \beta^{(0)} \in [0, \pi)$ such that

$$\mathrm{dom}(H_\beta) = \mathrm{dom}(H^{(0)}_{\beta^{(0)}}) \tag{4.77}$$

and denote the Friedrichs extensions of $\dot{H}$ and $\dot{H}^{(0)}$ by H_{α_F} and $H^{(0)}_{\alpha_F^{(0)}}$, respectively. In particular, since $V \in \mathcal{B}(\mathcal{H})$ this implies

$$\mathrm{dom}(H_{\alpha_F}) = \mathrm{dom}(H^{(0)}_{\alpha_F^{(0)}}). \tag{4.78}$$

Throughout the remainder of this section, the subscript F indicates the Friedrichs extension of $\dot{H}^{(0)}$ and $\dot{H}$ and we choose $\alpha = \alpha_F$ ($\alpha^{(0)} = \alpha_F^{(0)}$) in (4.65), (4.74), etc. We recall (cf., e.g., [23], [36]) that α_F for the Friedrichs extension H_{α_F} of $\dot{H}$ (and similarly $\alpha_F^{(0)}$ for the Friedrichs extension $H^{(0)}_{\alpha_F^{(0)}}$ of $\dot{H}^{(0)}$) is uniquely characterized by

$$\lim_{z \downarrow -\infty} m_{\alpha_F}(z) = -\infty. \tag{4.79}$$

Next, taking into account (4.63), (4.77), and (4.78), we recall the exponential Herglotz representations (cf. also [50]),

$$\ln(m_{\alpha_F}(z) + \cot(\beta - \alpha_F)) = c_{\alpha_F,\beta} + \int_{\mathbb{R}} d\lambda\, ((\lambda - z)^{-1} - \lambda(\lambda^2+1)^{-1})\eta_{\alpha_F,\beta}(\lambda), \tag{4.80}$$

$$\begin{aligned} &\ln(m^{(0)}_{\alpha_F^{(0)}}(z) + \cot(\beta^{(0)} - \alpha_F^{(0)})) \\ &\quad = c_{\alpha_F^{(0)},\beta^{(0)}} + \int_{\mathbb{R}} d\lambda\, ((\lambda - z)^{-1} - \lambda(\lambda^2+1)^{-1})\eta^{(0)}_{\alpha_F^{(0)},\beta^{(0)}}(\lambda), \end{aligned} \tag{4.81}$$

$$0 \leq \eta_{\alpha_F,\beta}(\lambda), \eta^{(0)}_{\alpha_F^{(0)},\beta^{(0)}}(\lambda) \leq 1 \text{ for a.e. } \lambda \in \mathbb{R}. \tag{4.82}$$

Combining the paragraph following (3.28) with (3.29), (4.63), (4.66) and (4.80), one verifies that $\eta_{\alpha_F,\beta}(\lambda)$ represents the Krein spectral shift function for the pair (H_{α_F}, H_β) (and analogously in the unperturbed case).

The following result links $m_{\alpha_F}(z)$ and $m^{(0)}_{\alpha_F^{(0)}}(z)$.

Lemma 4.10. *Suppose $z<0$, $|z|$ sufficiently large. Then*

$$\frac{d}{dz}m_{\alpha_F}(z) \underset{z\downarrow -\infty}{=} c^2\frac{d}{dz}m^{(0)}_{\alpha_F^{(0)}}(z) - c^2\frac{d}{dz}(u_+^{(0)}(z),Vu_+^{(0)}(z))_{\mathcal{H}} + O(|z|^{-2}), \tag{4.83}$$

$$m_{\alpha_F}(z) \underset{z\downarrow -\infty}{=} c^2 m^{(0)}_{\alpha_F^{(0)}}(z) + C_F - c^2(u_+^{(0)}(z),Vu_+^{(0)}(z))_{\mathcal{H}} + O(|z|^{-1}), \tag{4.84}$$

where

$$C_F = c^2\cot(\beta^{(0)}-\alpha_F^{(0)}) - \cot(\beta-\alpha_F). \tag{4.85}$$

Proof. Using (4.66), (4.73),

$$(H_{\alpha_F}-z)^{-1}u_+(z) = (H_{\alpha_F}-i)(H_{\alpha_F}-z)^{-2} = \frac{d}{dz}u_+(z), \tag{4.86}$$

the resolvent equation

$$(H_{\alpha_F}-z)^{-1} = (H^{(0)}_{\alpha_F^{(0)}}-z)^{-1} - (H^{(0)}_{\alpha_F^{(0)}}-z)^{-1}V(H_{\alpha_F}-z)^{-1}, \quad z\in\mathbb{C}\backslash\mathbb{R}, \tag{4.87}$$

and

$$\|u_+^{(0)}(z)\|_{\mathcal{H}} \underset{z\downarrow -\infty}{=} O(1), \tag{4.88}$$

one verifies (4.83). Equation (4.84) then follows upon integrating (4.83). The integration constant C_F can be determined by a somewhat lengthy perturbation argument as follows. For brevity we will temporarily use the following short-hand notations,

$$M(z)=m_{\alpha_F}(z), \quad m(z)=m^{(0)}_{\alpha_F^{(0)}}(z), \quad v(z)=(u_+^{(0)}(z),Vu_+^{(0)}(z))_{\mathcal{H}},$$

$$\gamma=\cot(\beta-\alpha_F), \quad \delta=\cot(\beta^{(0)}-\alpha_F^{(0)}). \tag{4.89}$$

First we claim

$$\lim_{z\downarrow-\infty} z^{-2}m(z)^2/m'(z)=0. \tag{4.90}$$

Since none of the spectral measures $d\mu_\beta(\lambda)$, $\beta\in[0,\pi)$ associated with the Herglotz representation of $m_\beta(z)$ in (4.62) is a finite measure on $\mathbb{R}$, one obtains from $m'(z)/(m(z)+\delta)^2 = ((-(m(z)+\delta)^{-1}))'$

$$z^2m'(z)(m(z)+\delta)^{-2} = \int_{\mathbb{R}} d\mu_{\beta_0}(\lambda)\, z^2(\lambda-z)^{-2} \uparrow +\infty \text{ as } z\downarrow-\infty \tag{4.91}$$

for some $\beta_0\in[0,\pi)$.

Next we will show that

$$(d/dz)\ln((M(z)+\gamma)/(m(z)+\delta)) \tag{4.92}$$

$$= \int_{\mathbb{R}} d\lambda\,(\lambda-z)^{-2}(\eta_{\alpha_F,\beta}(\lambda) - \eta^{(0)}_{\alpha_F^{(0)},\beta^{(0)}}(\lambda)) \tag{4.93}$$

$$= \operatorname{tr}((H_{\alpha_F}-z)^{-1} - (H_\beta-z)^{-1} - (H^{(0)}_{\alpha_F^{(0)}}-z)^{-1} + (H^{(0)}_{\beta^{(0)}}-z)^{-1}) \tag{4.94}$$

$$\underset{z\downarrow-\infty}{=} O(z^{-2}). \tag{4.95}$$

While (4.92)–(4.94) are clear from (4.63), (4.80), and (4.81), we need to prove the asymptotic relation (4.95). The difference of the first and the third resolvent as well as the difference of the second and fourth resolvent under the trace in (4.94) is clearly of $O(z^{-2})$ in norm using the resolvent equation and the fact that V is a bounded operator. On the other hand, the operator under the trace in (4.94) is the difference of two rank-one operators by (4.63) and hence at most of rank two. Hence the trace norm of the operator under the trace in (4.94) is also of order $O(z^{-2})$ as $z \downarrow -\infty$.

Integrating (4.92) taking into account (4.95) then proves that

$$m(z)/M(z) = O(1) \text{ and } M(z)/m(z) = O(1) \text{ as } z \downarrow -\infty. \tag{4.96}$$

Next we abbreviate

$$D(z) = (d/dz)\ln((M(z)+\gamma)/(m(z)+\delta)) \tag{4.97}$$

and compute (cf. (4.83))

$$\begin{aligned} D(z) &= \frac{M'(z)(m(z)+\delta) - m'(z)(M(z)+\gamma)}{(M(z)+\gamma)(m(z)+\delta)} \\ &= \frac{(c^2m'(z)+r(z))(m(z)+\delta) - m'(z)(M(z)+\gamma)}{(M(z)+\gamma)(m(z)+\delta)} \\ &= \frac{m'(z)}{(M(z)+\gamma)(m(z)+\delta)}(c^2(m(z)+\delta) - (M(z)+\gamma)) + \frac{r(z)}{M(z)+\gamma}, \end{aligned} \tag{4.98}$$

where

$$r(z) = -v'(z) + O(z^{-2}) = o(|m'(z)/m(z)|) \text{ as } z \downarrow -\infty \tag{4.99}$$

by taking into account

$$m(z) = o(|z|) \text{ as } z \downarrow -\infty \tag{4.100}$$

and

$$v'(z) = O(|m'(z)/z|) \text{ as } z \downarrow -\infty, \tag{4.101}$$

which in turn follows from (4.66), (4.86), the fact that V is a bounded operator, and $\|(H^{(0)}_{\alpha_F^{(0)}} - z)^{-1}\| = O(|z|^{-1})$ as $z \downarrow -\infty$. Thus,

$$\begin{aligned} &(m(z)^2/m'(z))D(z) \\ &= \frac{m(z)^2}{(M(z)+\gamma)(m(z)+\delta)}(c^2(m(z)+\delta) - (M(z)+\gamma)) \\ &\quad + \frac{m(z)^2 r(z)}{m'(z)(M(z)+\gamma)} \\ &= \frac{m(z)^2}{(M(z)+\gamma)(m(z)+\delta)}(c^2(m(z)+\delta) - (M(z)+\gamma)) + o(1) \\ &= -(m(z)/M(z))((M(z)+\gamma) - c^2(m(z)+\delta))) + o(1) \\ &= o(1) \text{ as } z \downarrow -\infty, \end{aligned} \tag{4.102}$$

by (4.90) and (4.95). This implies

$$\lim_{z\downarrow -\infty}((M(z)+\gamma) - c^2(m(z)+\delta)) = 0 \tag{4.103}$$

by (4.96) and hence proves (4.84) and (4.85). □

Our principal asymptotic result then reads as follows.

Theorem 4.11.

$$\begin{aligned} &\int_{\mathbb{R}} d\lambda\,(\lambda-z)^{-2}(\eta_{\alpha_F}(\lambda)-\eta^{(0)}_{\alpha_F^{(0)}}(\lambda)) \\ &\underset{z\downarrow-\infty}{=} -\frac{d}{dz}\bigg(\frac{(u_+^{(0)}(z),Vu_+^{(0)}(z))_{\mathcal{H}}}{m^{(0)}_{\alpha_F^{(0)}}(z)+\cot(\beta^{(0)}-\alpha_F^{(0)})}\bigg)+o(|z|^{-2}) \end{aligned} \tag{4.104}$$

and

$$\overline{\lim_{z\downarrow-\infty}}\int_{\mathbb{R}} d\lambda\, z^2(\lambda-z)^{-2}(\eta_{\alpha_F}(\lambda)-\eta^{(0)}_{\alpha_F^{(0)}}(\lambda)) \text{ exists.} \tag{4.105}$$

Proof. Differentiating (4.80) and (4.81) with respect to z, taking into account (4.83)–(4.85) yields

$$\begin{aligned} &\int_{\mathbb{R}} d\lambda\,(\lambda-z)^{-2}(\eta_{\alpha_F}(\lambda)-\eta^{(0)}_{\alpha_F^{(0)}}(\lambda)) \\ &\underset{z\downarrow-\infty}{=} \frac{(d/dz)m^{(0)}_{\alpha_F^{(0)}}(z)-(d/dz)(u_+^{(0)}(z),Vu_+^{(0)}(z))_{\mathcal{H}}+O(|z|^{-2})}{m^{(0)}_{\alpha_F^{(0)}}(z)+\cot(\beta^{(0)}-\alpha_F^{(0)})-(u_+^{(0)}(z),Vu_+^{(0)}(z))_{\mathcal{H}}+O(|z|^{-1})} \\ &\quad -\frac{(d/dz)m^{(0)}_{\alpha_F^{(0)}}(z)}{m^{(0)}_{\alpha_F^{(0)}}(z)+\cot(\beta^{(0)}-\alpha_F^{(0)})}. \end{aligned} \tag{4.106}$$

In order to verify (4.104) we need to estimate various terms. For brevity we will again temporarily use the short-hand notations introduced in (4.89). Thus, (4.106) becomes

$$\begin{aligned} &\frac{m'(z)-v'(z)+O(z^{-2})}{m(z)+\delta-v(z)+O(|z|^{-1})}-\frac{m'(z)}{m(z)+\delta} \\ &=-(d/dz)(v(z)/(m(z)+\delta))+O(|m(z)^{-1}z^{-2}|) \\ &\quad +O(|z^{-1}m'(z)m(z)^{-2}|)+O(|m'(z)v(z)^2m(z)^{-3}|) \\ &=-(d/dz)(v(z)/(m(z)+\delta))+o(z^{-2}) \text{ as } z\downarrow-\infty \end{aligned} \tag{4.107}$$

and we need to verify the last line in (4.107) and the claim (4.105). By (4.79), one concludes

$$O(|m(z)^{-1}z^{-2}|)=o(z^{-2}) \text{ as } z\downarrow-\infty. \tag{4.108}$$

Next, using

$$v(z)=O(|m'(z)|) \text{ as } z\downarrow-\infty \tag{4.109}$$

(cf. (4.66)), one obtains

$$O(|m'(z)v(z)^2m(z)^{-3}|)=O(|m'(z)^3m(z)^{-3}|)=O(|z|^{-3}) \text{ as } z\downarrow-\infty \tag{4.110}$$

since

$$m'(z)m(z)^{-1}=O(|z|^{-1}) \text{ as } z\downarrow-\infty. \tag{4.111}$$

Relation (4.111) is shown as follows. Since $-m'(z)(m(z)+\delta)^{-1}=(\ln(-(m(z)+\delta)^{-1})'$, and $-(m(z)+\delta)^{-1}$ (being distinct from the Friedrichs m-function) belongs to some measure $d\mu_{\beta_0}(\lambda)$ in (4.62) with $\int_{\mathbb{R}} d\mu_{\beta_0}(\lambda)(1+|\lambda|)^{-1}<\infty$, one concludes from [2] that also $\int_{\mathbb{R}} d\lambda\, \xi_{\beta_0}(\lambda)(1+|\lambda|)^{-1} < \infty$ in the corresponding exponential Herglotz representation of $-(m(z)+\delta)^{-1}$ (cf. (4.81)) and hence

$$-zm'(z)(m(z)+\delta)^{-1} = \int_{\mathbb{R}} d\lambda\, (-z)(\lambda - z)^{-2}\xi_{\beta_0}(\lambda) = O(1) \text{ as } z \downarrow -\infty. \tag{4.112}$$

Next, we note

$$O(|z^{-1}m'(z)m(z)^{-2}|) = O(|zm'(z)m(z)^{-1}|)O(|z^{-2}m(z)^{-1}|) = o(z^{-2}) \text{ as } z \downarrow -\infty \tag{4.113}$$

by (4.79) and (4.111) which proves (4.104).

To prove (4.105) one estimates

$$v'(z)m(z)^{-1} = O(|z^{-1}m'(z)m(z)^{-1}|) = O(z^{-2}) \text{ as } z \downarrow -\infty \tag{4.114}$$

using (4.101) and (4.111). Similarly,

$$v(z)m'(z)m(z)^{-2} = O(|m'(z)^2 m(z)^{-2}|) = O(z^{-2}) \text{ as } z \downarrow -\infty \tag{4.115}$$

by (4.111). This completes the proof. □

Next we will show that the abstract asymptotic result (4.106) contains concrete trace formulas for one-dimensional Schrödinger operators first derived in [35] (see also [26], [27], [29], [30]), and hence can be viewed as an abstract approach to trace formulas.

To make the connection with Schrödinger operators on the real line we choose $\mathcal{H} = L^2(\mathbb{R}; dx)$, pick a $y \in \mathbb{R}$, and identify V with the real-valued potential $V(x)$ assuming

$$V \in L^\infty(\mathbb{R}; dx) \cap C((y-\varepsilon, y+\varepsilon)) \text{ for some } \varepsilon > 0. \tag{4.116}$$

Similarly, we identify (in obvious notation) $\dot{H}$, $\dot{H}^*$, $H_{\pi/2}$, H_{α_F} with

$$\begin{aligned} &\dot{H}_y = -d^2/dx^2 + V, \\ &\operatorname{dom}(\dot{H}_y) = \{g \in L^2(\mathbb{R}; dx) \,|\, g, g' \in AC_{\text{loc}}(\mathbb{R});\ \lim_{\varepsilon \downarrow 0} g(y \pm \varepsilon) = 0;\ g'' \in L^2(\mathbb{R}; dx)\}, \end{aligned} \tag{4.117}$$

$$\begin{aligned} &\dot{H}_y^* = -d^2/dx^2 + V, \\ &\operatorname{dom}(\dot{H}_y^*) = \{g \in L^2(\mathbb{R}; dx) \,|\, g \in AC_{\text{loc}}(\mathbb{R}), g' \in AC_{\text{loc}}(\mathbb{R}\backslash\{y\});\ g'' \in L^2(\mathbb{R}; dx)\}, \end{aligned} \tag{4.118}$$

$$\begin{aligned} &H_{y,\pi/2} = -d^2/dx^2 + V, \\ &\operatorname{dom}(H_{y,\pi/2}) = \{g \in L^2(\mathbb{R}; dx) \,|\, g, g' \in AC_{\text{loc}}(\mathbb{R});\ g'' \in L^2(\mathbb{R}; dx)\} = H^{2,2}(\mathbb{R}), \end{aligned} \tag{4.119}$$

$$\begin{aligned} &H_{y,F} = -d^2/dx^2 + V, \\ &\operatorname{dom}(H_{y,F}) = \{g \in L^2(\mathbb{R}; dx) \,|\, g \in AC_{\text{loc}}(\mathbb{R}), g' \in AC_{\text{loc}}(\mathbb{R}\backslash\{y\});\ \lim_{\varepsilon \downarrow 0} g(y \pm \varepsilon) = 0; \\ &\hspace{9cm} g'' \in L^2(\mathbb{R}; dx)\}, \end{aligned} \tag{4.120}$$

respectively. (We note that $H_{y,\pi/2}$ is actually independent of $y \in \mathbb{R}$.) The corresponding unperturbed operators $\dot{H}_y^{(0)}$, $\dot{H}_y^{(0)*}$, $H_{y,\pi/2}^{(0)}$, $H_{y,F}^{(0)}$ are then defined as in (4.116)–(4.120) setting $V(x) = 0$, for all $x \in \mathbb{R}$.

Denoting by $G(z,x,x')$ the Green's function of $H_{y,\pi/2}$, that is,

$$G(z,x,x') = (H_{y,\pi/2}-z)^{-1}(x,x'), \quad z\in\mathbb{C}\backslash\mathbb{R},\ x,x'\in\mathbb{R}, \tag{4.121}$$

and observing that

$$G^{(0)}(z,x,x') = (H^{(0)}_{y,\pi/2}-z)^{-1}(x,x') = i2^{-1/2}z^{-1/2}\exp(iz^{1/2}|x-x'|), \quad z\in\mathbb{C}\backslash\mathbb{R},\ x,x'\in\mathbb{R}, \tag{4.122}$$

explicit computations then yield the following results for $z<0$, $|z|$ sufficiently large:

$$u_+(z,x) = G(z,x,y)/\|G(i,\cdot,y)\|_{\mathcal{H}}, \quad u_+^{(0)}(z,x) = 2^{-5/4}iz^{-1/2}\exp(iz^{1/2}|x-y|), \tag{4.123}$$

$$\tan(\alpha_F) = -\mathrm{Re}(G(i,y,y))/\mathrm{Im}(G(i,y,y)), \quad \alpha_F^{(0)} = 3\pi/4, \quad \beta=\beta^{(0)}=\pi/2, \tag{4.124}$$

$$\|u_+(z)\|^2_{\mathcal{H}} = \mathrm{Im}(G(z,y,y))/\mathrm{Im}(z), \quad \|u_+^{(0)}(z)\|^2_{\mathcal{H}} = 2^{-1/2}iz^{-1/2}, \tag{4.125}$$

$$(u_+^{(0)}(z), Vu_+^{(0)}(z))_{\mathcal{H}} = 2^{-1/2}iz^{-1/2}V(y)+o(|z|^{-1/2}), \tag{4.126}$$

$$(d/dz)(u_+^{(0)}(z), Vu_+^{(0)}(z))_{\mathcal{H}} = -2^{-3/2}iz^{-3/2}V(y)+o(|z|^{-3/2}), \tag{4.127}$$

$$m^{(0)}_{y,F}(z) = i(2z)^{1/2}+1, \quad \eta^{(0)}_{\alpha_F^{(0)}}(\lambda) = \begin{cases} 1/2, & \lambda>0, \\ 1, & \lambda<0, \end{cases} \tag{4.128}$$

$$(d/dz)(\ln(m^{(0)}_{y,F}(z) - (u_+^{(0)}(z), Vu_+^{(0)}(z))_{\mathcal{H}})) - (2z)^{-1} \underset{z\downarrow-\infty}{=} 2^{-1}V(y)z^{-2}+o(|z|^{-2}). \tag{4.129}$$

Moreover, one computes for $z\in\mathbb{C}\backslash\mathbb{R}$,

$$\begin{aligned} m_{y,\pi/2}(z) &= z+(1+z^2)(\mathrm{Im}(G(i,y,y)))^{-1}(G(i,\cdot,y),(H_{y,\pi/2}-z)^{-1}G(i,\cdot,y))_{\mathcal{H}} \\ &= (G(z,y,y)-\mathrm{Re}(G(i,y,y)))/\mathrm{Im}(G(i,y,y)), \end{aligned} \tag{4.130}$$

$$\begin{aligned} m_{y,\alpha_F}(z) &= z+(1+z^2)(\mathrm{Im}(G(i,y,y)))^{-1}(G(i,\cdot,y),(H_{y,\alpha_F}-z)^{-1}G(i,\cdot,y))_{\mathcal{H}} \\ &= (-G(z,y,y)^{-1}|G(i,y,y)|^2+\mathrm{Re}(G(i,y,y)))/\mathrm{Im}(G(i,y,y)). \end{aligned} \tag{4.131}$$

Combining (4.104) and (4.123)–(4.128), identifying $\eta_{\alpha_F}(\lambda)$, $\eta^{(0)}_{\alpha_F^{(0)}}(\lambda)$ with $\eta_{\alpha_F}(\lambda,y)$, $\eta^{(0)}_{\alpha_F^{(0)}}(\lambda)$, then yields the trace formula

$$V(y) = \lim_{z\downarrow-\infty} 2\int_{\mathbb{R}} d\lambda\, z^2(\lambda-z)^{-2}(\eta_{\alpha_F}(\lambda,y)-\eta^{(0)}_{\alpha_F^{(0)}}(\lambda)). \tag{4.132}$$

Since by (4.124) and (4.131),

$$m_{y,\alpha_F}(z)+\tan(\alpha_F) = -G(z,y,y)^{-1}/\mathrm{Im}(G(i,y,y)), \tag{4.133}$$

one can use the exponential Herglotz representation of $G(z,y,y)$, that is,

$$\ln(G(z,y,y)) = d(y)+\int_{\mathbb{R}} d\lambda\,((\lambda-z)^{-1}-\lambda(\lambda^2+1)^{-1})\xi(\lambda,y), \tag{4.134}$$

to rewrite the trace formula (4.132) in the form originally obtained in [30], [35],

$$V(y) = E_0 + \lim_{z\downarrow -\infty} \int_{E_0}^{\infty} d\lambda\, z^2(\lambda - z)^{-2}(1 - 2\xi(\lambda, y)), \quad E_0 = \inf(\mathrm{spec}(H_{y,\pi/2})). \tag{4.135}$$

Here we used the elementary facts

$$\xi(\lambda, y) = 1 - \eta_{y,\alpha_F}(\lambda), \quad \xi^{(0)}(\lambda) = 1 - \eta^{(0)}_{\alpha_F^{(0)}}(\lambda) = \begin{cases} 1/2, & \lambda > 0, \\ 0, & \lambda < 0. \end{cases} \tag{4.136}$$

Of course this formalism is not restricted to the case where $\mathrm{def}\,(\dot{H}) = (1, 1)$. The analogous construction in the case $\mathrm{def}\,(\dot{H}) = (n, n)$, $n \in \mathbb{N}$, then yields an abstract approach to matrix-valued trace formulas. This formalism is applicable to matrix Schrödinger operators and reproduces the matrix-valued trace formula analog of (4.135) first derived in [28]. To actually prove a formula of the type (4.135) for a matrix-valued $n \times n$ potential $V(x)$ using this abstract framework, one then factors the imaginary part of the $n \times n$ matrix $\mathrm{Im}(-G(i, y, y)^{-1})$ into

$$\mathrm{Im}(-G(i, y, y)^{-1}) = S(y)^* S(y) \tag{4.137}$$

for some $n \times n$ matrix $S(y)$ and uses relations of the type

$$G(z, y, y) = -(S(y)^* M_{y,\alpha_F}(z) S(y) + \mathrm{Re}(-G(i, y, y)^{-1}))^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{4.138}$$

where $M_{y,\alpha_F}(z)$ denotes the $n \times n$ Donoghue M-matrix (cf. [31], [34], [36]) for the coresponding matrix-valued Friedrichs extension H_{α_F} of $\dot{H}$ and matrix-valued exponential Herglotz representations of the type

$$\begin{aligned} &\ln(-G(z, y, y)^{-1}) = C(y) + \int_{\mathbb{R}} d\lambda\, ((\lambda - z)^{-1} - \lambda(\lambda^2 + 1)^{-1})\Upsilon(\lambda, y), \\ &C(y) = C(y)^*, \quad 0 \le \Upsilon(\lambda, y) \le I_n \text{ for a.e. } \lambda \in \mathbb{R}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \end{aligned} \tag{4.139}$$

Since the actual details are a bit involved, we will return to this topic elsewhere [32].

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