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An abstract approach to weak convergence of spectral shift functions and applications to multi-dimensional Schrödinger operators

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Dedicated to the memory of Nigel J. Kalton (1946–2010)

Abstract. We study the manner in which a sequence of spectral shift functions $\xi(\cdot; H_j, H_{0,j})$ associated with abstract pairs of self-adjoint operators $(H_j, H_{0,j})$ in Hilbert spaces $\mathcal{H}_j$, $j \in \mathbb{N}$, converges to a limiting spectral shift function $\xi(\cdot; H, H_0)$ associated with a pair (H, H_0) in the limiting Hilbert space $\mathcal{H}$ as $j \to \infty$ (mimicking the infinite volume limit in concrete applications to multi-dimensional Schrödinger operators).

Our techniques rely on a Fredholm determinant approach combined with certain measure theoretic facts. In particular, we show that prior vague convergence results for spectral shift functions in the literature actually extend to the notion of weak convergence. More precisely, in the concrete case of multi-dimensional Schrödinger operators on a sequence of domains Ω_j exhausting $\mathbb{R}^n$ as $j \to \infty$, we extend the convergence of associated spectral shift functions from vague to weak convergence and also from Dirichlet boundary conditions to more general self-adjoint boundary conditions on $\partial\Omega_j$.

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Contents

1. Introduction

We are interested in the manner in which a sequence of spectral shift functions for abstract pairs of self-adjoint operators $(H_j, H_{0,j})$ in Hilbert spaces $\mathcal{H}_j$, $j \in \mathbb{N}$, converges to a limiting spectral shift function associated with a pair (H, H_0) in a limiting Hilbert space $\mathcal{H}$ as $j \to \infty$ (mimicking the infinite volume limit in concrete situations). As a concrete application we explicitly treat the case of multi-dimensional Schrödinger on bounded domains $\Omega_j \subset \mathbb{R}^n$, $n \in \mathbb{N}$, exhausting $\mathbb{R}^n$ as $j \to \infty$, with various boundary conditions on $\partial\Omega_j$, $j \in \mathbb{N}$ (we primarily focus on the cases $1 \leqslant n \leqslant 3$).

An exhaustive treatment of the special one-dimensional case appeared in [37].

Before we focus on the abstract situation discussed in this paper, it is appropriate to briefly survey the known results in this area. Consider self-adjoint Schrödinger operators H_j and $H_{0,j}$ in $L^2((-j, j)^n; d^n x)$, $n \in \mathbb{N}$, $n \geqslant 2$, generated by the differential expression $-\Delta + V$ and $-\Delta$ on $(-j, j)^n$, respectively, with Dirichlet boundary conditions on $\partial(-j, j)^n$, where $0 \leqslant V \in L^\infty(\mathbb{R}^n; d^n x)$ is supported in $(-j, j)^n$, for $j \in \mathbb{N}$ sufficiently large, and nonzero a.e. Denoting by $\xi(\lambda; H_j, H_{0,j})$ for a.e. $\lambda \in \mathbb{R}$, the spectral shift function associated with the pair $(H_j, H_{0,j})$ (cf. [77], Chapter 8), normalized to be zero in a neighborhood of $-\infty$, Kirsch [52] showed in 1987 that (perhaps, somewhat unexpectedly), for any $\lambda > 0$,

$$\sup_{j \in \mathbb{N}} |\xi(\lambda; H_j, H_{0,j})| = \infty. \tag{1.1}$$

Moreover, denoting by H and H_0 the corresponding self-adjoint Schrödinger operators in $L^2(\mathbb{R}^n; d^n x)$ generated by the differential expression $-\Delta + V$ and $-\Delta$ on $\mathbb{R}^n$, respectively, one cannot expect pointwise a.e. convergence (or convergence in measure) of $\xi(\cdot; H_j, H_{0,j})$ (or of a subsequence thereof) to $\xi(\cdot; H, H_0)$ in the infinite volume limit $j \to \infty$ by the following elementary argument: For a.e. $\lambda > 0$, $\xi(\lambda; H, H_0)$ is a continuous function with respect to λ, related to the determinant of the underlying fixed energy scattering matrix. Yet $\xi(\cdot; H_j, H_{0,j})$, as a difference of eigenvalue counting functions corresponding to the number of eigenvalues (counting multiplicity) of H_j and $H_{0,j}$, respectively, is integer-valued and hence cannot possibly converge a.e. to a non-constant continuous function as $j \to \infty$. In particular, this argument applies to the one-dimensional context (in which case $\xi(\lambda; H, H_0) \to 0$ as $\lambda \to \infty$).

Having ruled out pointwise a.e. convergence of spectral shift functions in the infinite volume limit $j \to \infty$ in all space dimensions, it becomes clear that one has to invoke the concept of certain generalized limits. Indeed, in 1995, Geisler, Kostrykin, and Schrader [31] proved for potentials $V \in \ell^1(L^2(\mathbb{R}^3; d^3 x))$ (a Birman–Solomyak space, cf., e.g., [74], Chapter 4) that for all $\lambda \in \mathbb{R}$,

$$\lim_{j \to \infty} \int_{(-\infty, \lambda]} \xi(\lambda'; H_j, H_{0,j}) d\lambda' = \int_{(-\infty, \lambda]} \xi(\lambda'; H, H_0) d\lambda'. \tag{1.2}$$

Since H_j and $H_{0,j}$ are bounded from below uniformly with respect to $j \in \mathbb{N}$, the limiting relation (1.2) involving distribution functions of the spectral shift measures is equivalent to vague convergence of the latter as observed in [49], Proposition 4.3.

In the one-dimensional half-line context, Borovyk and Makarov [14] (see also Borovyk [13]) proved in 2009 that for potentials $V \in L^1((0,\infty); (1+|x|)dx)$ real-valued, and denoting by H_R the self-adjoint Schrödinger operator in $L^2((0,R); dx)$ and H the corresponding self-adjoint Schrödinger operator in $L^2((0,\infty); dx)$, both with Dirichlet boundary conditions (and otherwise maximally defined or defined in terms of quadratic forms), and analogously for $H_{0,R}$ and H_0 in the unperturbed case $V = 0$, the following vague limit holds:

$$\lim_{R\to\infty} \int_{\mathbb{R}} \xi(\lambda; H_R, H_{0,R}) d\lambda\, g(\lambda) = \int_{\mathbb{R}} \xi(\lambda; H, H_0) d\lambda\, g(\lambda), \quad g \in C_0(\mathbb{R}). \tag{1.3}$$

In addition, they proved that the following Cesàro limit,

$$\lim_{R\to\infty} \frac{1}{R} \int_0^R \xi(\lambda; H_r, H_{0,r}) dr = \xi(\lambda; H, H_0), \quad \lambda \in \mathbb{R}\backslash(\sigma_{\mathrm{d}}(H) \cup \{0\}) \tag{1.4}$$

exists (and the limit in (1.4) extends to $\lambda = 0$ if H has no zero energy resonance).

Returning to the case of multi-dimensional boxes $[-R, R]^n$, Hislop and Müller [44] (see also [45]) proved a result going somewhat beyond vague convergence in 2010. More precisely, assuming a real-valued background potential $V^{(0)}$ satisfying $V_-^{(0)} \in K(\mathbb{R}^n)$, $V_+^{(0)} \in K_{\mathrm{loc}}(\mathbb{R}^n)$ and a potential $0 \leqslant V \in K_{\mathrm{loc}}(\mathbb{R}^n)$, $\mathrm{supp}(V)$ compact (cf. [2] and [73] for the definition of (local) Kato classes), they show that

$$\begin{aligned} &\lim_{R\to\infty} \int_{\mathbb{R}} \xi(\lambda; H_{0,R} + V^{(0)} + V, H_{0,R} + V^{(0)}) d\lambda\, f(\lambda) \\ &\quad = \int_{\mathbb{R}} \xi(\lambda; H_0 + V^{(0)} + V, H_0 + V^{(0)}) d\lambda\, f(\lambda) \end{aligned} \tag{1.5}$$

for any $f \in C_0(\mathbb{R})$, and for any $f = \chi_J$, were $J \subset \mathbb{R}$ is a finite interval. In addition, they derived a weaker version than the Cesáro limit in (1.4) in the multi-dimensional context. More precisely, they proved that for every sequence of lengths $\{L_j\}_{j\in\mathbb{N}} \subset (0,\infty)$ with $\lim_{j\to\infty} L_j = \infty$, there exists a subsequence $\{j_k\}_{k\in\mathbb{N}} \subset \mathbb{N}$ with $\lim_{k\to\infty} j_k = \infty$, such that for every subsequence $\{k_\ell\}_{\ell\in\mathbb{N}} \subset \mathbb{N}$ with $\lim_{\ell\to\infty} k_\ell = \infty$,

$$\begin{aligned} &\lim_{L\to\infty} \frac{1}{L} \sum_{\ell=1}^{L} \xi(\lambda; H^{(0)}_{L_{j_{k_\ell}}} + V^{(0)} + V, H^{(0)}_{L_{j_{k_\ell}}} + V^{(0)}) \\ &\quad \leqslant \xi(\lambda; H_0 + V^{(0)} + V, H_0 + V^{(0)}) \end{aligned} \tag{1.6}$$

for (Lebesgue) a.e. $\lambda \in \mathbb{R}$.

Before describing our results we should mention that spectral shift functions feature prominently in the context of eigenvalue counting functions and hence in the context of the integrated density of states. We refer, for instance, to [18], [19], [43], [47], [48], [54], [55], [56], [62], and the references cited therein. For bounds on the spectral shift function we refer to [19], [47], [48], and [75].

In Section 2 we collect basic properties of spectral shift functions used in the bulk of this paper. In Section 3 we prove our principal abstract result, the convergence of a sequence of spectral shift functions $\xi(\cdot; H_j, H_{0,j})$ associated with pairs of self-adjoint operators $(H_j, H_{0,j})$ in Hilbert spaces $\mathcal{H}_j$, $j \in \mathbb{N}$, to the limiting spectral shift function $\xi(\cdot; H, H_0)$ associated with the pair (H, H_0) in a limiting Hilbert space $\mathcal{H}$ as $j \to \infty$, thus mimicking the infinite volume limit in concrete situations. Finally, in Section 4 we provide detailed applications to Schrödinger operators in dimensions $n = 1, 2, 3$ in the case of Dirichlet boundary conditions and sketch extensions to higher dimensions $n \geqslant 4$ and Robin boundary conditions.

Finally, we briefly summarize some of the notation used in this paper. Let $\mathcal{H}$ be a separable complex Hilbert space, $(\cdot, \cdot)_{\mathcal{H}}$ the scalar product in $\mathcal{H}$ (linear in the second argument), and $I_{\mathcal{H}}$ the identity operator in $\mathcal{H}$. Next, let T be a linear operator mapping (a subspace of) a Hilbert space into another, with $\operatorname{dom}(T)$ and $\ker(T)$ denoting the domain and kernel (i.e., null space) of T. The closure of a closable operator S is denoted by $\overline{S}$. The resolvent set, spectrum, essential spectrum, discrete spectrum, and resolvent set of a closed linear operator in $\mathcal{H}$ will be denoted by $\rho(\cdot)$, $\sigma(\cdot)$, $\sigma_{\rm ess}(\cdot)$, $\sigma_{\rm d}(\cdot)$, and $\rho(\cdot)$, respectively. The Banach space of bounded (resp., compact) linear operators on $\mathcal{H}$ is denoted by $\mathcal{B}(\mathcal{H})$ (resp., $\mathcal{B}_\infty(\mathcal{H})$). The corresponding ℓ^p-based trace ideals will be denoted by $\mathcal{B}_p(\mathcal{H})$, $p > 0$. The trace of trace class operators in $\mathcal{H}$ is denoted by $\operatorname{tr}_{\mathcal{H}}(\cdot)$, modified Fredholm determinants are abbreviated by $\det_{p,\mathcal{H}}(I_{\mathcal{H}} + \cdot)$, $p \in \mathbb{N}$ (the subscript p being omitted in the trace class case $p = 1$).

The form sum (resp., difference) of two self-adjoint operators A and W will be denoted by $A +_q W$ (resp., $A -_q W = A +_q (-W)$).

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2. Basic facts on spectral shift functions

In this preparatory section we succinctly summarize properties of the spectral shift function as needed in the bulk of this paper (for details on this material we refer to [11], [77], Chapter 8, [78], and [79], Section 0.9 and Chapters 4, 5, and 9).

We start with the following basic assumptions.

Hypothesis 2.1. *Suppose A and B are self-adjoint operators in $\mathcal{H}$ with A bounded from below.*

(i) *Assume that B can be written as the form sum of A and a self-adjoint operator W in $\mathcal{H}$*

$$B = A +_q W, \tag{2.1}$$

where W can be factorized into

$$W = W_1^* W_2, \tag{2.2}$$

such that

$$\operatorname{dom}(W_j) \supseteq \operatorname{dom}(|A|^{1/2}), \quad j = 1, 2. \tag{2.3}$$

(ii) *Suppose that for some (and hence for all) $z \in \rho(A)$,*

$$W_2(A - zI_{\mathcal{H}})^{-1/2}, \overline{(A - zI_{\mathcal{H}})^{-1/2} W_1^*} \in \mathcal{B}_2(\mathcal{H}), \tag{2.4}$$

and that

$$\lim_{z \downarrow -\infty} \|\overline{W_2(A - zI_{\mathcal{H}})^{-1} W_1^*}\|_{\mathcal{B}_1(\mathcal{H})} = 0. \tag{2.5}$$

Given Hypothesis 2.1(i), one observes that

$$\operatorname{dom}(|B|^{1/2}) = \operatorname{dom}(|A|^{1/2}), \tag{2.6}$$

and that the resolvent of B can be written as (cf., e.g., the detailed discussion in [33] and the references therein)

$$\begin{aligned} &(B - zI_{\mathcal{H}})^{-1} \\ &\quad = (A - zI_{\mathcal{H}})^{-1} \\ &\qquad - \overline{(A - zI_{\mathcal{H}})^{-1} W_1^*} [I_{\mathcal{H}} + \overline{W_2(A - zI_{\mathcal{H}})^{-1} W_1^*}]^{-1} W_2 (A - zI_{\mathcal{H}})^{-1}, \end{aligned} \tag{2.7}$$

for all $z \in \rho(B) \cap \rho(A)$. In particular, B is bounded from below in $\mathcal{H}$ and one concludes that for some (and hence for all) $z \in \rho(B) \cap \rho(A)$,

$$[(B - zI_{\mathcal{H}})^{-1} - (A - zI_{\mathcal{H}})^{-1}] \in \mathcal{B}_1(\mathcal{H}). \tag{2.8}$$

Moreover, assuming the full Hypothesis 2.1 one infers that (cf. [38])

$$\begin{aligned} &\operatorname{tr}_{\mathcal{H}}((B - zI_{\mathcal{H}})^{-1} - (A - zI_{\mathcal{H}})^{-1}) \\ &\quad = -\frac{d}{dz} \ln(\det_{\mathcal{H}}(\overline{(B - zI_{\mathcal{H}})^{1/2} (A - zI_{\mathcal{H}})^{-1} (B - zI_{\mathcal{H}})^{1/2}})) \\ &\quad = -\frac{d}{dz} \ln(\det_{\mathcal{H}}(I_{\mathcal{H}} + \overline{W_2(A - zI_{\mathcal{H}})^{-1} W_1^*})), \end{aligned} \tag{2.9}$$

for all $z \in \rho(B) \cap \rho(A)$.

In addition, Hypothesis 2.1 guarantees the existence of the real-valued spectral shift function $\xi(\cdot; B, A)$ satisfying

$$\operatorname{tr}_{\mathcal{H}}((B - zI_{\mathcal{H}})^{-1} - (A - zI_{\mathcal{H}})^{-1}) = -\int_{\mathbb{R}} \frac{\xi(\lambda; B, A)\, d\lambda}{(\lambda - z)^2}, \tag{2.10}$$

for all $z \in \rho(B) \cap \rho(A)$, and

$$\xi(\lambda; B, A) = 0, \quad \lambda < \inf(\sigma(B), \sigma(A)), \tag{2.11}$$

$$\xi(\cdot; B, A) \in L^1(\mathbb{R}; (\lambda^2 + 1)^{-1} d\lambda). \tag{2.12}$$

Moreover, for a large class of functions f, for instance, any f such that $\hat{f}(\cdot) \in L^1(\mathbb{R}; (|p| + 1)dp)$, one infers that $[f(B) - f(A)] \in \mathcal{B}_1(\mathcal{H})$ and

$$\operatorname{tr}_{\mathcal{H}}(f(B) - f(A)) = \int_{\mathbb{R}} f'(\lambda)\, \xi(\lambda; B, A)\, d\lambda. \tag{2.13}$$

This applies, in particular, to powers of the resolvent, where $f(\cdot) = (\cdot - z)^{-n}$, $n \in \mathbb{N}$, and we refer to [77], Chapter 8, for more details.

Throughout this manuscript we assume that the normalization (2.11) is applied.

For subsequent purpose we summarize the results (2.9) and (2.10) as

$$\begin{aligned} &\operatorname{tr}_{\mathcal{H}}((B - zI_{\mathcal{H}})^{-1} - (A - zI_{\mathcal{H}})^{-1}) \\ &\quad = -\int_{\mathbb{R}} \frac{\xi(\lambda; B, A)\, d\lambda}{(\lambda - z)^2} \\ &\quad = -\frac{d}{dz} \ln(\det_{\mathcal{H}}(I_{\mathcal{H}} + \overline{W_2(A - zI_{\mathcal{H}})^{-1} W_1^*})), \end{aligned} \tag{2.14}$$

for all $z \in \rho(B) \cap \rho(A)$. Here $\det_{\mathcal{H}}(\cdot)$ denotes the Fredholm determinant (cf. [40], Chapter IV, [69], and [74], Chapter 3).

We also note the following monotonicity result.

$$\begin{aligned} &\text{If } B \geqslant A \text{ (resp., } B \leqslant A) \text{ in the sense of quadratic forms,} \\ &\text{then } \xi(\lambda; B, A) \geqslant 0 \text{ (resp., } \xi(\lambda; B, A) \leqslant 0). \end{aligned} \tag{2.15}$$

Here, $B \geqslant A$ is meant in the sense of quadratic forms, that is,

$$\begin{aligned} &\operatorname{dom}(|A|^{1/2}) \supseteq \operatorname{dom}(|B|^{1/2}), \\ &(|B|^{1/2} f,\ \operatorname{sgn}(B)|B|^{1/2} f)_{\mathcal{H}} \\ &\qquad \geqslant (|A|^{1/2} f,\ \operatorname{sgn}(A)|A|^{1/2} f)_{\mathcal{H}}, \quad f \in \operatorname{dom}(|B|^{1/2}). \end{aligned} \tag{2.16}$$

Next, suppose that the self-adjoint operator C in $\mathcal{H}$ can be written as the form sum of B and a self-adjoint operator Q in $\mathcal{H}$, $C = B +_q Q$, where Q can be factored as $Q = Q_1 Q_2$, with Q, Q_1, and Q_2 satisfying the assumptions of W, W_1, and W_2 in Hypotheses 2.1. Then the formula

$$\xi(\lambda; C, A) = \xi(\lambda; C, B) + \xi(\lambda; B, A) \tag{2.17}$$

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

Finally, we mention the connection between $\xi(\cdot; B, A)$ and the Fredholm determinant in (2.9),

$$\xi(\lambda; B, A) = \pi^{-1} \lim_{\varepsilon \downarrow 0} \operatorname{Im}(\ln(I_{\mathcal{H}} + \overline{W_2(A - (\lambda + i\varepsilon) I_{\mathcal{H}})^{-1} W_1^*})), \tag{2.18}$$

for a.e. $\lambda \in \mathbb{R}$, choosing the branch of $\ln(\det_{\mathcal{H}}(\cdot))$ on $\mathbb{C}_+$ such that

$$\lim_{|\operatorname{Im}(z)| \to \infty} \ln(\det_{\mathcal{H}}(I_{\mathcal{H}} + \overline{W_2(A - z I_{\mathcal{H}})^{-1} W_1^*})) = 0. \tag{2.19}$$

For applications to multi-dimensional Schrödinger operators the framework in Hypothesis 2.1 is not sufficiently general and the trace class assumption, (2.4), needs to be replaced by a weaker Hilbert–Schmidt-type hypothesis as detailed next.

Hypothesis 2.2. *Suppose A and B are self-adjoint operators in $\mathcal{H}$ with A bounded from below.*

(i) *Assume that B can be written as the form sum of A and a self-adjoint operator W in $\mathcal{H}$*

$$B = A +_q W, \tag{2.20}$$

where W can be factorized into

$$W = W_1^* W_2, \tag{2.21}$$

such that

$$\operatorname{dom}(W_j) \supseteq \operatorname{dom}(|A|^{1/2}), \quad j = 1, 2. \tag{2.22}$$

(ii) *Assume that, for some (and hence for all) $z \in \rho(A)$,*

$$W_2(A - z I_{\mathcal{H}})^{-1}, \ \overline{(A - z I_{\mathcal{H}})^{-1} W_1^*} \in \mathcal{B}_2(\mathcal{H}), \tag{2.23}$$

$$\overline{W_2(A - z I_{\mathcal{H}})^{-1} W_1^*} \in \mathcal{B}_2(\mathcal{H}), \tag{2.24}$$

and

$$\lim_{z \downarrow -\infty} \|\overline{W_2(A - z I_{\mathcal{H}})^{-1} W_1^*}\|_{\mathcal{B}_2(\mathcal{H})} = 0. \tag{2.25}$$

(iii) *Suppose that*

$$\operatorname{tr}_{\mathcal{H}}(\overline{(A - zI_{\mathcal{H}})^{-1} W (A - zI_{\mathcal{H}})^{-1}}) = \eta'(z), \quad z \in \rho(A), \tag{2.26}$$

where $\eta(\cdot)$ has normal limits, denoted by $\eta(\lambda + i0)$, for a.e. $\lambda \in \mathbb{R}$.

Then (2.6)–(2.8), (2.10)–(2.17) remain valid, but (2.9), (2.18), and (2.19) need to be amended as follows.

Theorem 2.3. *Assume Hypothesis 2.2. Then*

$$\begin{aligned} \xi(\lambda; B, A) = {} & \pi^{-1} \operatorname{Im}(\ln(\det_{2,\mathcal{H}}(I_{\mathcal{H}} + \overline{W_2 (A - (\lambda + i0) I_{\mathcal{H}})^{-1} W_1^*}))) \\ & + \pi^{-1} \operatorname{Im}(\eta(\lambda + i0)) + c \end{aligned} \tag{2.27}$$

for a.e. $\lambda \in \mathbb{R}$. Here $c \in \mathbb{R}$ has to be chosen in accordance with the normalization (2.11).

Proof. First, one notes that

$$\begin{aligned} & |\operatorname{tr}_{\mathcal{H}}(\overline{(A - zI_{\mathcal{H}})^{-1} W (A - zI_{\mathcal{H}})^{-1}})| \\ & \quad = |\operatorname{tr}_{\mathcal{H}}(\overline{W_2 (A - zI_{\mathcal{H}})^{-2} W_1^*})| \\ & \quad \leq \|\overline{(A - zI_{\mathcal{H}})^{-1} W (A - zI_{\mathcal{H}})^{-1}}\|_{\mathcal{B}_1(\mathcal{H})} \\ & \quad \leq |z|^{-1} \|W_1 (A - \bar{z} I_{\mathcal{H}})^{-1/2}\|_{\mathcal{B}(\mathcal{H})} \, \|W_2 (A - zI_{\mathcal{H}})^{-1/2}\|_{\mathcal{B}(\mathcal{H})} \\ & \quad \underset{z \downarrow -\infty}{=} C |z|^{-1}. \end{aligned} \tag{2.28}$$

Next, one recalls that

$$\begin{aligned} & (B - zI_{\mathcal{H}})^{-1} - (A - zI_{\mathcal{H}})^{-1} + (A - zI_{\mathcal{H}})^{-1} W (A - zI_{\mathcal{H}})^{-1} \\ & \quad = (A - zI_{\mathcal{H}})^{-1} W_1^* [I_{\mathcal{H}} + \overline{W_2 (A - zI_{\mathcal{H}})^{-1} W_1^*}]^{-1} \\ & \qquad \times \overline{W_2 (A - zI_{\mathcal{H}})^{-1} W_1^*} W_2 (A - zI_{\mathcal{H}})^{-1}, \end{aligned} \tag{2.29}$$

for all $z \in \rho(B) \cap \rho(A)$, and hence (cf. [77], Section 1.7) that

$$\begin{aligned} & \operatorname{tr}_{\mathcal{H}}((B - zI_{\mathcal{H}})^{-1} - (A - zI_{\mathcal{H}})^{-1} + \overline{(A - zI_{\mathcal{H}})^{-1} W (A - zI_{\mathcal{H}})^{-1}}) \\ & \quad = \operatorname{tr}_{\mathcal{H}}([I_{\mathcal{H}} + \overline{W_2 (A - zI_{\mathcal{H}})^{-1} W_1^*}]^{-1} \overline{W_2 (A - zI_{\mathcal{H}})^{-1} W_1^*} \\ & \qquad \times [(d/dz) W_2 (A - zI_{\mathcal{H}})^{-1}]), \\ & \quad = -\frac{d}{dz} \ln(\det_{2,\mathcal{H}}(I_{\mathcal{H}} + \overline{W_2 (A - zI_{\mathcal{H}})^{-1} W_1^*})), \end{aligned} \tag{2.30}$$

for all $z \in \rho(B) \cap \rho(A)$. Consequently,

$$\begin{aligned}
&\mathrm{tr}_{\mathcal{H}}((B - zI_{\mathcal{H}})^{-1} - (A - zI_{\mathcal{H}})^{-1}) \\
&\quad = -\int_{\mathbb{R}} \frac{\xi(\lambda; B, A)d\lambda}{(\lambda - z)^2} \\
&\quad = -\frac{d}{dz}\int_{\mathbb{R}} \xi(\lambda; B, A)d\lambda\Big(\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1}\Big) \\
&\quad = -\mathrm{tr}_{\mathcal{H}}(\overline{(A - zI_{\mathcal{H}})^{-1}W(A - zI_{\mathcal{H}})^{-1}}) \\
&\qquad\qquad - \frac{d}{dz}\ln(\det_{2,\mathcal{H}}(I_{\mathcal{H}} + \overline{W_2(A - zI_{\mathcal{H}})^{-1}W_1^*}), \\
&\quad = -\eta'(z) - \frac{d}{dz}\ln(\det_{2,\mathcal{H}}(I_{\mathcal{H}} + \overline{W_2(A - zI_{\mathcal{H}})^{-1}W_1^*}),
\end{aligned} \tag{2.31}$$

for all $z \in \rho(B) \cap \rho(A)$, and hence

$$\begin{aligned}
&\int_{\mathbb{R}} \xi(\lambda; B, A)d\lambda\Big(\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1}\Big) \\
&\qquad = \eta(z) + \ln(\det_{2,\mathcal{H}}(I_{\mathcal{H}} + \overline{W_2(A - zI_{\mathcal{H}})^{-1}W_1^*})) + C,
\end{aligned} \tag{2.32}$$

for all $z \in \rho(B) \cap \rho(A)$, and for some $C \in \mathbb{C}$. Taking $z < 0$, $|z|$ sufficiently large, (2.25) and (2.28) actually yield

$$C \in \mathbb{R}. \tag{2.33}$$

Moreover, (2.32) demonstrates that $\det_{2,\mathcal{H}}(I_{\mathcal{H}} + \overline{W_2(A - zI_{\mathcal{H}})^{-1}W_1^*})$ has normal limits $z \to \lambda + i0$ for a.e. $\lambda \in \mathbb{R}$. The Stieltjes inversion formula (cf., e.g., [5]) then yields (2.27). □

We note that the analog of (2.27) was discussed in [54], Theorems 1.59 and 1.61, in the concrete context of multi-dimensional Schrödinger operators (an additional sign-definiteness of potentials was assumed for $n \geqslant 4$).

For subsequent purpose we record the analog of (2.14) (cf. (2.31))

$$\begin{aligned}
&\mathrm{tr}_{\mathcal{H}}((B - zI_{\mathcal{H}})^{-1} - (A - zI_{\mathcal{H}})^{-1}) \\
&\quad = -\int_{\mathbb{R}} \frac{\xi(\lambda; B, A)d\lambda}{(\lambda - z)^2} \\
&\quad = -\mathrm{tr}_{\mathcal{H}}(\overline{(A - zI_{\mathcal{H}})^{-1}W(A - zI_{\mathcal{H}})^{-1}}) \\
&\qquad\qquad - \frac{d}{dz}\ln(\det_{2,\mathcal{H}}(I_{\mathcal{H}} + \overline{W_2(A - zI_{\mathcal{H}})^{-1}W_1^*}),
\end{aligned} \tag{2.34}$$

for all $z \in \rho(B) \cap \rho(A)$.

For pertinent literature on (modified) Fredholm determinants and associated trace formulas we refer, for instance, to [6], [40], Chapter IV, [54], Section 1,6 [69], [74], Chapter 9, [77], Section 1.7, [78], and [79], Chapters 3 and 9.

We conclude this preparatory section by analyzing the high-energy limiting assumptions (2.5) and (2.25). We start by recalling the following standard convergence property for trace ideals.

Lemma 2.4. *Let $p \in [1, \infty)$ and assume that $R, R_n, T, T_n \in \mathcal{B}(\mathcal{H})$, $n \in \mathbb{N}$, satisfy* s-$\lim_{n\to\infty} R_n = R$ *and* s-$\lim_{n\to\infty} T_n = T$ *and that $S, S_n \in \mathcal{B}_p(\mathcal{H})$, $n \in \mathbb{N}$, satisfy $\lim_{n\to\infty} \|S_n - S\|_{\mathcal{B}_p(\mathcal{H})} = 0$. Then $\lim_{n\to\infty} \|R_n S_n T_n^* - RST^*\|_{\mathcal{B}_p(\mathcal{H})} = 0$.*

This follows, for instance, from [41], Theorem 1, from [74], p, 28–29, or from [77], Lemma 6.1.3, with a minor additional effort (taking adjoints, etc.).

Lemma 2.5. *Let $p \in [1, \infty)$ and assume that A is self-adjoint and bounded from below in $\mathcal{H}$. Let W_j, $j = 1, 2$, be densely defined linear operators in $\mathcal{H}$ satisfying*

$$\operatorname{dom}(W_j) \supseteq \operatorname{dom}(|A|^{1/2}), \quad j = 1, 2, \tag{2.35}$$

and for some $z_0 \in \rho(A)$,

$$\overline{W_2(A - z_0 I_{\mathcal{H}})^{-1} W_1^*} \in \mathcal{B}_p(\mathcal{H}). \tag{2.36}$$

In addition, suppose one of the following three conditions holds:

$$W_1(A - \bar{z}_0 I_{\mathcal{H}})^{-1/2} \in \mathcal{B}_q(\mathcal{H}), \quad W_2(A - z_0 I_{\mathcal{H}})^{-1/2} \in \mathcal{B}_r(\mathcal{H}), \tag{2.37}$$

$$W_1(A - \bar{z}_0 I_{\mathcal{H}})^{-1/2} \in \mathcal{B}_p(\mathcal{H}), \quad W_2(A - z_0 I_{\mathcal{H}})^{-1/2} \in \mathcal{B}(\mathcal{H}), \tag{2.38}$$

$$W_1(A - \bar{z}_0 I_{\mathcal{H}})^{-1/2} \in \mathcal{B}(\mathcal{H}), \quad W_2(A - z_0 I_{\mathcal{H}})^{-1/2} \in \mathcal{B}_p(\mathcal{H}), \tag{2.39}$$

for $\dfrac{1}{q} + \dfrac{1}{r} = \dfrac{1}{p}$, $q, r \in [1, \infty)$. Then

$$\begin{aligned} &\lim_{z\downarrow-\infty} \|\overline{W_2(A - zI_{\mathcal{H}})^{-1} W_1^*}\|_{\mathcal{B}_p(\mathcal{H})} \\ &\quad = \lim_{|\operatorname{Im}(z)|\to\infty} \|\overline{W_2(A - zI_{\mathcal{H}})^{-1} W_1^*}\|_{\mathcal{B}_p(\mathcal{H})} = 0, \end{aligned} \tag{2.40}$$

and hence

$$\begin{aligned} &\lim_{z\downarrow-\infty} \det_{p,\mathcal{H}}(I_{\mathcal{H}} + \overline{W_2(A - zI_{\mathcal{H}})^{-1} W_1^*}) \\ &\quad = \lim_{|\operatorname{Im}(z)|\to\infty} \det_{p,\mathcal{H}}(I_{\mathcal{H}} + \overline{W_2(A - zI_{\mathcal{H}})^{-1} W_1^*}) = 1. \end{aligned} \tag{2.41}$$

Proof. We start with the identity

$$\begin{aligned}
&\overline{W_2(A - zI_{\mathcal{H}})^{-1}W_1^*} \\
&\quad = \overline{W_2[(A - z_0 I_{\mathcal{H}})^{-1} + (z - z_0)(A - z_0 I_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{-1}]W_1^*} \\
&\quad = W_2(A - z_0 I_{\mathcal{H}})^{-1/2}[I_{\mathcal{H}} + (z - z_0)(A - zI_{\mathcal{H}})^{-1}][W_1(A - \overline{z_0} I_{\mathcal{H}})^{-1/2}]^*,
\end{aligned} \tag{2.42}$$

for all $z \in \rho(A)$. Combining (2.42) with the fact that

$$\begin{aligned}
&\operatorname*{s-lim}_{z \downarrow -\infty} [I_{\mathcal{H}} + (z - z_0)(A - zI_{\mathcal{H}})^{-1}] \\
&\quad = \operatorname*{s-lim}_{|\mathrm{Im}(z)| \to \infty} [I_{\mathcal{H}} + (z - z_0)(A - zI_{\mathcal{H}})^{-1}] = 0,
\end{aligned} \tag{2.43}$$

$$\begin{aligned}
&\operatorname*{s-lim}_{z \downarrow -\infty} [I_{\mathcal{H}} + (z - z_0)(A - zI_{\mathcal{H}})^{-1}]^* \\
&\quad = \operatorname*{s-lim}_{|\mathrm{Im}(z)| \to \infty} [I_{\mathcal{H}} + (z - z_0)(A - zI_{\mathcal{H}})^{-1}]^* = 0,
\end{aligned} \tag{2.44}$$

then permits the application of Lemma 2.4 to conclude that

$$\|[I_{\mathcal{H}} + (z - z_0)(A - zI_{\mathcal{H}})^{-1}][W_1(A - \overline{z_0} I_{\mathcal{H}})^{-1/2}]^*\|_{\mathcal{B}_r(\mathcal{H})} \longrightarrow 0 \tag{2.45}$$

as $z \downarrow -\infty$ and also as $|\mathrm{Im}(z)| \to \infty$. This implies (2.38) in the case (2.37) is assumed. The cases where (2.38) or (2.39) are assumed are analogous. Continuity of $\det_{p,\mathcal{H}}(I + T)$ as a function of T with respect to the $\|\cdot\|_{\mathcal{B}_p(\mathcal{H})}$-norm, $p \in [1, \infty)$, yields (2.39). □

The argument in the proof of Lemma 2.5 is analogous to the proof of [77], Lemma 8.1.1, where the stronger relative trace class assumption $W_1^* W_2 (A - z_0)^{-1} \in \mathcal{B}_1(\mathcal{H})$ is made.

3. An abstract approach to convergence of spectral shift functions

In this section we prove our principal abstract result, the convergence of a sequence of spectral shift functions $\xi(\cdot; H_j, H_{0,j})$ associated with pairs of self-adjoint operators $(H_j, H_{0,j})$ in Hilbert spaces $\mathcal{H}_j$, $j \in \mathbb{N}$, to the limiting spectral shift function $\xi(\cdot; H, H_0)$ associated with the pair (H, H_0) in a limiting Hilbert space $\mathcal{H}$ as $j \to \infty$ (mimicking the infinite volume limit in concrete situations).

We start with a precise list of our assumptions employed throughout this section.

Hypothesis 3.1. *Let $\mathcal{H}$ be a complex, separable Hilbert space.*

(i) *Assume that $\{P_j\}_{j\in\mathbb{N}}$ is a sequence of orthogonal projections in $\mathcal{H}$, strongly converging to the identity in $\mathcal{H}$,*

$$\operatorname*{s-lim}_{j\to\infty} P_j = I_{\mathcal{H}}, \tag{3.1}$$

and introduce the sequence of closed subspaces $\mathcal{H}_j = P_j\mathcal{H}$, $j \in \mathbb{N}$, of $\mathcal{H}$.

(ii) *Let H_0 be a self-adjoint operator in $\mathcal{H}$, and for each $j \in \mathbb{N}$, let $H_{0,j}$ be self-adjoint operators in $\mathcal{H}_j$. In addition, suppose that H_0 is bounded from below in $\mathcal{H}$, and for each $j \in \mathbb{N}$, $H_{0,j}$ are bounded from below in $\mathcal{H}_j$.*

(iii) *Suppose that V_1, and V_2 are closed operators in $\mathcal{H}$, and for each $j \in \mathbb{N}$, assume that $V_{1,j}$, and $V_{2,j}$ are closed operators in $\mathcal{H}_j$ such that*

$$\operatorname{dom}(V_1) \cap \operatorname{dom}(V_2) \supseteq \operatorname{dom}(H_0), \tag{3.2}$$

$$\operatorname{dom}(V_{1,j}) \cap \operatorname{dom}(V_{2,j}) \supseteq \operatorname{dom}(H_{0,j}), \quad j \in \mathbb{N}, \tag{3.3}$$

and

$$\overline{V_2(H_0 - zI_{\mathcal{H}})^{-1}V_1^*},\ \overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1}V_{1,j}^*} \oplus 0 \in \mathcal{B}_1(\mathcal{H}), \tag{3.4}$$

$$V_2(H_0 - zI_{\mathcal{H}})^{-1},\ V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1} \oplus 0 \in \mathcal{B}_2(\mathcal{H}), \tag{3.5}$$

$$\overline{(H_0 - zI_{\mathcal{H}})^{-1}V_1^*},\ \overline{(H_{0,j} - zI_{\mathcal{H}_j})^{-1}V_{1,j}^*} \oplus 0 \in \mathcal{B}_2(\mathcal{H}), \tag{3.6}$$

for all $j \in \mathbb{N}$ and for some (and hence for all) $z \in \mathbb{C}\backslash\mathbb{R}$. In addition, assume that

$$\begin{aligned} &\lim_{z\downarrow-\infty} \|[\overline{V_2(H_0 - zI_{\mathcal{H}})^{-1}V_1^*}\|_{\mathcal{B}_1(\mathcal{H})} = 0, \\ &\lim_{z\downarrow-\infty} \|[\overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1}V_{1,j}^*} \oplus 0]\|_{\mathcal{B}_1(\mathcal{H})} = 0, \quad j \in \mathbb{N}. \end{aligned} \tag{3.7}$$

Here we used the orthogonal decomposition of $\mathcal{H}$ into

$$\mathcal{H} = \mathcal{H}_j \oplus \mathcal{H}_j^{\perp}, \quad j \in \mathbb{N}. \tag{3.8}$$

(iv) *Assume that for some (and hence for all) $z \in \mathbb{C}\backslash\mathbb{R}$,*

$$\operatorname*{s-lim}_{j\to\infty} \Big[(H_{0,j} - zI_{\mathcal{H}_j})^{-1} \oplus \frac{-1}{z} I_{\mathcal{H}_j^{\perp}}\Big] = (H_0 - zI_{\mathcal{H}})^{-1}. \tag{3.9}$$

(v) *Suppose that for some (and hence for all) $z \in \mathbb{C}\backslash\mathbb{R}$,*

$$\begin{aligned} &\lim_{j\to\infty} \|[\overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1}V_{1,j}^*} \oplus 0] - \overline{V_2(H_0 - zI_{\mathcal{H}})^{-1}V_1^*}\|_{\mathcal{B}_1(\mathcal{H})} \\ &\quad = 0, \end{aligned} \tag{3.10}$$

$$\lim_{j\to\infty} \|[V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1} \oplus 0] - V_2(H_0 - zI_{\mathcal{H}})^{-1}\|_{\mathcal{B}_2(\mathcal{H})} = 0, \tag{3.11}$$

$$\lim_{j\to\infty} \|\overline{[(H_{0,j} - zI_{\mathcal{H}_j})^{-1}V_{1,j}^*} \oplus 0] - \overline{(H_0 - z)^{-1}V_1^*}\|_{\mathcal{B}_2(\mathcal{H})} = 0. \tag{3.12}$$

(vi) *Suppose that*

$$\begin{aligned} (V_2 f, V_1 g)_{\mathcal{H}} &= (V_1 f, V_2 g)_{\mathcal{H}}, \quad f, g \in \operatorname{dom}(V_1) \cap \operatorname{dom}(V_2), \\ (V_{2,j} f, V_{1,j} g)_{\mathcal{H}} &= (V_{1,j} f, V_{2,j} g)_{\mathcal{H}}, \ f, g \in \operatorname{dom}(V_{1,j}) \cap \operatorname{dom}(V_{2,j}), \end{aligned} \tag{3.13}$$

for all $j \in \mathbb{N}$.

Following Kato [50], Hypothesis 3.1, permits one to define the self-adjoint operator H in $\mathcal{H}$, and for each $j \in \mathbb{N}$, the self-adjoint operators H_j in $\mathcal{H}_j$ via their resolvents (for $z \in \mathbb{C}\backslash\mathbb{R}$) by

$$\begin{aligned} &(H - zI_{\mathcal{H}})^{-1} \\ &\quad = (H_0 - zI_{\mathcal{H}})^{-1} \\ &\qquad - \overline{(H_0 - zI_{\mathcal{H}})^{-1}V_1^*}[I_{\mathcal{H}} + \overline{V_2(H_0 - zI_{\mathcal{H}})^{-1}V_1^*}]^{-1}V_2(H_0 - zI_{\mathcal{H}})^{-1}, \end{aligned} \tag{3.14}$$

$$\begin{aligned} &(H_j - zI_{\mathcal{H}_j})^{-1} \\ &\quad = (H_{0,j} - zI_{\mathcal{H}_j})^{-1} \\ &\qquad - \overline{(H_{0,j} - zI_{\mathcal{H}_j})^{-1}V_{1,j}^*}[I_{\mathcal{H}_j} + \overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1}V_{1,j}^*}]^{-1} \\ &\qquad\qquad \times V_{2,j}(H_0 - zI_{\mathcal{H}_j})^{-1}, \end{aligned} \tag{3.15}$$

for all $j \in \mathbb{N}$. Of course, both resolvent equations (3.14) and (3.15) extend by continuity to $\rho(H) \cap \rho(H_0)$ and $\rho(H_j) \cap \rho(H_{0,j})$, $j \in \mathbb{N}$, respectively.

Lemma 3.2. *Assume Hypothesis 3.1. Then*

$$\operatorname*{s-lim}_{j\to\infty} \Big[(H_j - zI_{\mathcal{H}_j})^{-1} \oplus \frac{-1}{z} I_{\mathcal{H}_j^\perp}\Big] = (H - zI_{\mathcal{H}})^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{3.16}$$

and

$$[(H - zI_{\mathcal{H}})^{-1} - (H_0 - zI_{\mathcal{H}})^{-1}] \in \mathcal{B}_1(\mathcal{H}), \quad z \in \rho(H) \cap \rho(H_0), \tag{3.17}$$

$$[(H_j - zI_{\mathcal{H}_j})^{-1} - (H_{0,j} - zI_{\mathcal{H}_j})^{-1}] \in \mathcal{B}_1(\mathcal{H}_j), \quad z \in \rho(H_j) \cap \rho(H_{0,j}), \ j \in \mathbb{N}. \tag{3.18}$$

Proof. To prove (3.16) it suffices to combine (3.9)–(3.12), (3.14), and (3.15). Similarly, (3.17) and (3.18) follow upon combining (3.4)–(3.6), (3.14) and (3.15). □

One notes that the trace class and Hilbert–Schmidt assumptions in (3.4)–(3.6) and (3.10)–(3.12) are by no means necessary for the proof of (3.16). In particular, $\mathcal{B}_1(\mathcal{H})$ or $\mathcal{B}_2(\mathcal{H})$ could be replaced by $\mathcal{B}(\mathcal{H})$ in all these places (and we will use a Hilbert–Schmidt assumption later in the context of Theorem 3.18).

Remark 3.3. We also note that if $H_{0,j} \geqslant c_0 I_{\mathcal{H}_j}$ for some $c_0 \in \mathbb{R}$ independent of $j \in \mathbb{N}$, and if

$$\lim_{z \downarrow -\infty} \|[\overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1} V_{1,j}^*} \oplus 0]\|_{\mathcal{B}(\mathcal{H})} = 0, \tag{3.19}$$

uniformly with respect to $j \in \mathbb{N}$, then (3.15) shows that also H_j are bounded from below, uniformly with respect to $j \in \mathbb{N}$, that is, $H_j \geqslant c I_{\mathcal{H}_j}$ for some $c \in \mathbb{R}$ independent of $j \in \mathbb{N}$.

Assuming Hypothesis 3.1, we now abbreviate by

$$\xi(\cdot) = \xi(\cdot; H, H_0), \quad \xi_j(\cdot) = \xi(\cdot; H_j, H_{0,j}), \quad j \in \mathbb{N}, \tag{3.20}$$

the Krein spectral shift functions corresponding to the pairs (H, H_0) in $\mathcal{H}$ and $(H_j, H_{0,j})$ in $\mathcal{H}_j$, respectively. Thus, for $z \in \mathbb{C}\backslash\mathbb{R}$,

$$\begin{aligned} \operatorname{tr}_{\mathcal{H}}((H - zI_{\mathcal{H}})^{-1} - (H_0 - zI_{\mathcal{H}})^{-1}) &= -\int_{\mathbb{R}} \frac{\xi(\lambda) d\lambda}{(\lambda - z)^2}, \\ \operatorname{tr}_{\mathcal{H}_j}((H_j - zI_{\mathcal{H}_j})^{-1} - (H_{0,j} - zI_{\mathcal{H}_j})^{-1}) &= -\int_{\mathbb{R}} \frac{\xi_j(\lambda) d\lambda}{(\lambda - z)^2}, \end{aligned} \tag{3.21}$$

with,

$$\xi, \xi_j \in L^1(\mathbb{R}; (1 + \lambda^2)^{-1} d\lambda), \quad j \in \mathbb{N}. \tag{3.22}$$

In addition, we introduce the perturbation determinants

$$\begin{aligned} D(z) &= \det_{\mathcal{H}}(I_{\mathcal{H}} + \overline{V_2(H_0 - zI_{\mathcal{H}})^{-1} V_1^*}), \quad z \in \rho(H) \cap \rho(H_0), \\ D_j(z) &= \det_{\mathcal{H}_j}(I_{\mathcal{H}_j} + \overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1} V_{1,j}^*}), \\ &\qquad z \in \rho(H_j) \cap \rho(H_{0,j}), \, j \in \mathbb{N}. \end{aligned} \tag{3.23}$$

We start with the following preliminary results.

Lemma 3.4. *Assume Hypothesis 3.1 and let $a, z \in \mathbb{C}\backslash\mathbb{R}$. Then*

$$\lim_{j \to \infty} \ln(D_j(z)/D_j(a)) = \ln(D(z)/D(a)), \tag{3.24}$$

$$\lim_{j \to \infty} \int_{\mathbb{R}} \frac{\xi_j(\lambda) d\lambda}{(\lambda - a)(\lambda - z)^n} = \int_{\mathbb{R}} \frac{\xi(\lambda) d\lambda}{(\lambda - a)(\lambda - z)^n}, \quad n \in \mathbb{N}. \tag{3.25}$$

Proof. The identities

$$\begin{aligned}
&\det_{\mathcal{H}_j}(I_{\mathcal{H}_j} + \overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1}V_{1,j}^*}) \\
&\quad = \det_{\mathcal{H}}((I_{\mathcal{H}_j} + \overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1}V_{1,j}^*}) \oplus I_{\mathcal{H}_j^\perp}) \\
&\quad = \det_{\mathcal{H}}(I_{\mathcal{H}} + (\overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1}V_{1,j}^*} \oplus 0)),
\end{aligned} \tag{3.26}$$

for all $j \in \mathbb{N}$, together with (3.10) and continuity of $\det_{\mathcal{H}}(I + A)$ as a function of A with respect to the trace norm $\|\cdot\|_{\mathcal{B}_1(\mathcal{H})}$, immediately yield

$$\lim_{j\to\infty} D_j(z) = D(z), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{3.27}$$

and hence the convergence in (3.24).

Applying (2.9), one verifies that for any $a, z \in \mathbb{C}\backslash\mathbb{R}$,

$$\ln(D(z)/D(a)) = (z-a)\int_{\mathbb{R}} \frac{\xi(\lambda)d\lambda}{(\lambda-a)(\lambda-z)}, \tag{3.28}$$

$$\ln(D_j(z)/D_j(a)) = (z-a)\int_{\mathbb{R}} \frac{\xi_j(\lambda)d\lambda}{(\lambda-a)(\lambda-z)}, \tag{3.29}$$

for all $j \in \mathbb{N}$.

To verify (3.25), we start with the basic identities (see, e.g., [77], Chapter 8)

$$\operatorname{tr}_{\mathcal{H}}((H_0 - zI_{\mathcal{H}})^{-n} - (H - zI_{\mathcal{H}})^{-n}) = n\int_{\mathbb{R}} \frac{\xi(\lambda)d\lambda}{(\lambda-z)^{n+1}}, \tag{3.30}$$

$$\operatorname{tr}_{\mathcal{H}_j}((H_{0,j} - zI_{\mathcal{H}_j})^{-n} - (H_j - zI_{\mathcal{H}_j})^{-n}) = n\int_{\mathbb{R}} \frac{\xi_j(\lambda)d\lambda}{(\lambda-z)^{n+1}}, \tag{3.31}$$

for all $j \in \mathbb{N}$, $n \in \mathbb{N}$, and $z \in \mathbb{C}\backslash\mathbb{R}$. Next we claim that

$$\begin{aligned}
&\lim_{j\to\infty} \operatorname{tr}_{\mathcal{H}_j}((H_{0,j} - zI_{\mathcal{H}_j})^{-n} - (H_j - zI_{\mathcal{H}_j})^{-n}) \\
&\quad = \operatorname{tr}_{\mathcal{H}}((H_0 - zI_{\mathcal{H}})^{-n} - (H - zI_{\mathcal{H}})^{-n}),
\end{aligned} \tag{3.32}$$

for all $n \in \mathbb{N}$ and $z \in \mathbb{C}\backslash\mathbb{R}$. To see this, one notes that

$$\begin{aligned}
&\operatorname{tr}_{\mathcal{H}_j}((H_{0,j} - zI_{\mathcal{H}_j})^{-n} - (H_j - zI_{\mathcal{H}_j})^{-n}) \\
&\quad = \operatorname{tr}_{\mathcal{H}}(((H_{0,j} - zI_{\mathcal{H}_j})^{-n} - (H_j - zI_{\mathcal{H}_j})^{-n}) \oplus 0) \\
&\quad = \operatorname{tr}_{\mathcal{H}}\Big[\Big((H_{0,j} - zI_{\mathcal{H}_j})^{-1} \oplus \frac{-1}{z} I_{\mathcal{H}_j^\perp}\Big)^n \\
&\qquad\qquad - \Big((H_j - zI_{\mathcal{H}_j})^{-1} \oplus \frac{-1}{z} I_{\mathcal{H}_j^\perp}\Big)^n\Big],
\end{aligned} \tag{3.33}$$

for all $n \in \mathbb{N}$ and $z \in \mathbb{C}\backslash\mathbb{R}$. Since the trace functional is continuous with respect to the $\mathcal{B}_1(\mathcal{H})$-norm, to verify (3.32), it suffices to prove that

$$\sum_{k=1}^{n} \Big((H_{0,j} - zI_{\mathcal{H}_j})^{-1} \oplus \frac{-1}{z} I_{\mathcal{H}_j^\perp}\Big)^{n-k} [(H_{0,j} - zI_{\mathcal{H}_j})^{-1} - (H_j - zI_{\mathcal{H}_j})^{-1} \oplus 0] \times \Big((H_j - zI_{\mathcal{H}_j})^{-1} \oplus \frac{-1}{z} I_{\mathcal{H}_j^\perp}\Big)^{k-1} \tag{3.34}$$

converges to

$$\sum_{k=1}^{n} (H_0 - zI_{\mathcal{H}})^{k-n} [(H_0 - zI_{\mathcal{H}})^{-1} - (H - zI_{\mathcal{H}})^{-1}](H - zI_{\mathcal{H}})^{1-k} \tag{3.35}$$

in $\mathcal{B}_1(\mathcal{H})$ as $j \to \infty$, since (3.34) is the operator under the trace on the r.h.s. of (3.33) and (3.35) is the operator under the trace on the r.h.s. of (3.32).[1]

By (3.9), one concludes that

$$\operatorname*{s-lim}_{j\to\infty} \Big((H_{0,j} - zI_{\mathcal{H}_j})^{-1} \oplus \frac{-1}{z} I_{\mathcal{H}_j^\perp}\Big)^{n-k} = (H_0 - zI_{\mathcal{H}})^{k-n}, \tag{3.36}$$

$$\operatorname*{s-lim}_{j\to\infty} \Big((H_j - zI_{\mathcal{H}_j})^{-1} \oplus \frac{-1}{z} I_{\mathcal{H}_j^\perp}\Big)^{k-1} = (H - zI_{\mathcal{H}})^{1-k}. \tag{3.37}$$

Thus, convergence of (3.34) to (3.35), will follow from Grümm's Theorem [41] (see also Lemma 2.4 and the discussion in [74], Chapter 2) if we can show that

$$\lim_{j\to\infty} \|[((H_{0,j} - zI_{\mathcal{H}_j})^{-1} - (H_j - zI_{\mathcal{H}_j})^{-1}) \oplus 0] - (H_0 - zI_{\mathcal{H}})^{-1} - (H - zI_{\mathcal{H}})^{-1}\|_{\mathcal{B}_1(\mathcal{H})} = 0. \tag{3.38}$$

The convergence in (3.38) follows readily from the identities

$$\begin{aligned} &((H_j - zI_{\mathcal{H}_j})^{-1} - (H_{0,j} - zI_{\mathcal{H}_j})^{-1}) \oplus 0 \\ &\quad = (\overline{(H_{0,j} - zI_{\mathcal{H}_j})^{-1} V_{1,j}^*} \oplus 0) \\ &\qquad \times ([I_{\mathcal{H}} + \overline{(V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1} V_{1,j}^*} \oplus 0)]^{-1} - (0 \oplus I_{\mathcal{H}_j^\perp})) \\ &\qquad \times (V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1} \oplus 0) \end{aligned} \tag{3.39}$$

and

$$\begin{aligned} &(H_0 - zI_{\mathcal{H}})^{-1} - (H - zI_{\mathcal{H}})^{-1} \\ &\quad = \overline{(H_0 - zI_{\mathcal{H}})^{-1} V_1^*}[I_{\mathcal{H}} + \overline{V_2(H_0 - zI_{\mathcal{H}})^{-1} V_1^*}]^{-1} V_2 (H_0 - zI_{\mathcal{H}})^{-1}. \end{aligned} \tag{3.40}$$

[1] Here we have made use of the identity $A^n - B^n = \sum_{k=1}^{n} A^{n-k}(A - B)B^{k-1}$.

Hypothesis (3.1) and relation (3.10) yield the strong convergence

$$\begin{aligned} &\operatorname*{s-lim}_{j\to\infty}([I_{\mathcal{H}} + (\overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1}V_{1,j}^*} \oplus 0)]^{-1} - (0 \oplus I_{\mathcal{H}_j^\perp})) \\ &\quad = [I + \overline{V_2(H_0 - zI_{\mathcal{H}})^{-1}V_1^*}]^{-1}. \end{aligned} \tag{3.41}$$

Therefore, (3.41) and (3.11) together with Grümm's Theorem [41] yield

$$\begin{aligned} \lim_{j\to\infty} &([I_{\mathcal{H}} + (\overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1}V_{1,j}^*} \oplus 0)]^{-1} \\ &\qquad - (0 \oplus I_{\mathcal{H}_j^\perp}))(V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1} \oplus 0) \\ &= [I + \overline{V_2(H_0 - zI_{\mathcal{H}})^{-1}V_1^*}]^{-1}V_2(H_0 - zI_{\mathcal{H}})^{-1} \quad \text{in } \mathcal{B}_2(\mathcal{H}). \end{aligned} \tag{3.42}$$

The convergence in (3.42) and (3.12) yields convergence of the r.h.s. of (3.39) to (3.40) in $\mathcal{B}_1(\mathcal{H})$, implying (3.38).

Employing (3.31), (3.30), and (3.38), we have shown that

$$\lim_{j\to\infty} \int_{\mathbb{R}} \frac{\xi_j(\lambda)d\lambda}{(\lambda - z)^{n+1}} = \int_{\mathbb{R}} \frac{\xi(\lambda)d\lambda}{(\lambda - z)^{n+1}}, \quad n \in \mathbb{N}, \tag{3.43}$$

so that (3.25) holds in the special case $a = z$. Thus, it remains to settle the case $z \neq a$.

For $z \neq a$ one notes that

$$\begin{aligned} \int_{\mathbb{R}} \frac{\xi_j(\lambda)d\lambda}{(\lambda - a)(\lambda - z)^{n+1}} &= \frac{1}{z - a}\left[\int_{\mathbb{R}} \frac{\xi_j(\lambda)d\lambda}{(\lambda - z)^{n+1}} - \int_{\mathbb{R}} \frac{\xi_j(\lambda)d\lambda}{(\lambda - a)(\lambda - z)^n}\right], \\ \int_{\mathbb{R}} \frac{\xi(\lambda)d\lambda}{(\lambda - a)(\lambda - z)^{n+1}} &= \frac{1}{z - a}\left[\int_{\mathbb{R}} \frac{\xi(\lambda)d\lambda}{(\lambda - z)^{n+1}} - \int_{\mathbb{R}} \frac{\xi(\lambda)d\lambda}{(\lambda - a)(\lambda - z)^n}\right], \end{aligned} \tag{3.44}$$

for $n \in \mathbb{N}$. Convergence in (3.25) now follows from (3.43) and the two identities in (3.44) via a simple induction on n. We emphasize that (3.24) yields the crucial first induction step, $n = 1$, since (3.24) implies, via (3.29) and (3.28), that

$$\lim_{j\to\infty} \int_{\mathbb{R}} \frac{\xi_j(\lambda)d\lambda}{(\lambda - a)(\lambda - z)} = \int_{\mathbb{R}} \frac{\xi(\lambda)d\lambda}{(\lambda - a)(\lambda - z)}, \quad z \neq a. \tag{3.45}$$

□

In the following we denote by $C_\infty(\mathbb{R})$ the space of continuous functions on $\mathbb{R}$ vanishing at infinity.

Lemma 3.5. *Let $f, f_j \in L^1(\mathbb{R}; d\lambda)$ and suppose that for some fixed $M > 0$, $\|f_j\|_{L^1(\mathbb{R};d\lambda)} \leq M$, $j \in \mathbb{N}$. If*

$$\begin{aligned} &\lim_{j\to\infty} \int_{\mathbb{R}} f_j(\lambda)d\lambda\, P((\lambda + i)^{-1}, (\lambda - i)^{-1}) \\ &\quad = \int_{\mathbb{R}} f(\lambda)d\lambda\, P((\lambda + i)^{-1}, (\lambda - i)^{-1}) \end{aligned} \tag{3.46}$$

for all polynomials $P(\cdot,\cdot)$ in two variables, then

$$\lim_{j\to\infty}\int_{\mathbb{R}} f_j(\lambda)d\lambda\, g(\lambda) = \int_{\mathbb{R}} f(\lambda)d\lambda\, g(\lambda), \quad g\in C_\infty(\mathbb{R}). \tag{3.47}$$

Proof. Let $\varepsilon>0$ and $g\in C_\infty(\mathbb{R})$. Since by a Stone–Weierstrass argument, polynomials in $(\lambda\pm i)^{-1}$ are dense in $C_\infty(\mathbb{R})$, there is a polynomial $P(\cdot,\cdot)$ in two variables such that writing

$$\mathcal{P}(\lambda) = P((\lambda+i)^{-1},(\lambda-i)^{-1}), \quad \lambda\in\mathbb{R}, \tag{3.48}$$

one concludes that

$$\|g-\mathcal{P}\|_{L^\infty(\mathbb{R};d\lambda)} \leqslant \frac{\varepsilon}{2[M+\|f\|_{L^1(\mathbb{R};d\lambda)}]}. \tag{3.49}$$

By (3.46), there exists an $N(\varepsilon)\in\mathbb{N}$ such that

$$\left|\int_{\mathbb{R}} f_j(\lambda)d\lambda\,\mathcal{P}(\lambda) - \int_{\mathbb{R}} f(\lambda)d\lambda\,\mathcal{P}(\lambda)\right| \leqslant \frac{\varepsilon}{2} \quad j\geqslant N(\varepsilon). \tag{3.50}$$

Therefore, if $j\geqslant N(\varepsilon)$,

$$\begin{aligned}
&\left|\int_{\mathbb{R}} f_j(\lambda)d\lambda\, g(\lambda) - \int_{\mathbb{R}} f(\lambda)d\lambda\, g(\lambda)\right| \\
&\quad\leqslant [\|f_j\|_{L^1(\mathbb{R};d\lambda)} + \|f\|_{L^1(\mathbb{R};d\lambda)}]\,\|g-\mathcal{P}\|_{L^\infty(\mathbb{R};d\lambda)} \\
&\qquad\qquad + \left|\int_{\mathbb{R}} f_j(\lambda)d\lambda\,\mathcal{P}(\lambda) - \int_{\mathbb{R}} f(\lambda)d\lambda\,\mathcal{P}(\lambda)\right| \\
&\quad\leqslant \varepsilon.
\end{aligned} \tag{3.51}$$

□

Next, we continue with some preparations needed to prove the principal results of this section. We start by recalling some basic notions regarding the convergence of positive measures (essentially following Bauer [8], Section 30). Denoting by $\mathcal{M}_+(E)$ the set of all *positive Radon measures* on a locally compact space E, and by

$$\mathcal{M}_+^b(E) = \{\mu\in\mathcal{M}_+(E) \mid \mu(E)<+\infty\}, \tag{3.52}$$

the set of all *finite* positive Radon measures on E, we note that in the special case $E=\mathbb{R}^n$, $n\in\mathbb{N}$, $\mathcal{M}_+^b(\mathbb{R}^n)$ represents the set of all finite positive Borel measures on $\mathbb{R}^n$.

If μ is a Radon measure, a point $x\in E$ is called an *atom* of μ if $\mu(\{x\})>0$.

In the following, $C_0(E)$ denotes the continuous functions on E with compact support, and $C_b(E)$ represents the bounded continuous functions on E.

Definition 3.6. Let E be a locally compact space.

(i) A sequence $\{\mu_j\}_{j\in\mathbb{N}} \subset \mathcal{M}_+(E)$ is said to be *vaguely convergent* to a Radon measure $\mu \in \mathcal{M}_+(E)$ if

$$\lim_{j\to\infty} \int_E d\mu_j \, g = \int_E d\mu \, g, \quad g \in C_0(E). \tag{3.53}$$

(ii) A sequence $\{\mu_j\}_{j\in\mathbb{N}} \subset \mathcal{M}_+^b(E)$ is said to be *weakly convergent* to $\mu \in \mathcal{M}_+^b(E)$ if

$$\lim_{j\to\infty} \int_E d\mu_j \, f = \int_E d\mu \, f, \quad f \in C_b(E). \tag{3.54}$$

(iii) A Borel set $B \subset E$ is called *boundaryless* with respect to the measure $\mu \in \mathcal{M}_+^b(E)$ (in short, *μ-boundaryless*), if the boundary ∂B of B has μ-measure equal to zero, $\mu(\partial B) = 0$.

Theorem 3.7 ([8], Theorem 30.8). *Suppose that the sequence $\{\mu_j\}_{j\in\mathbb{N}} \subset \mathcal{M}_+^b(E)$ converges vaguely to the measure $\mu \in \mathcal{M}_+^b(E)$. Then the following statements are equivalent.*

(i) *The sequence μ_j converges weakly to μ as $j \to \infty$.*

(ii) $\lim_{j\to\infty} \mu_j(E) = \mu(E)$.

(iii) *For every $\varepsilon > 0$ there exists a compact set K_ε of E such that*

$$\mu_j(E\backslash K_\varepsilon) \leqslant \varepsilon, \quad j \in \mathbb{N}. \tag{3.55}$$

Theorem 3.8 ([8], Theorem 30.12). *Suppose that the sequence $\{\mu_j\}_{j\in\mathbb{N}} \subset \mathcal{M}_+^b(E)$ converges weakly to $\mu \in \mathcal{M}_+^b(E)$. Then*

$$\lim_{j\to\infty} \int_E d\mu_j \, f = \int_E d\mu \, f \tag{3.56}$$

holds for every bounded Borel measurable function f that is μ-almost everywhere continuous on E. In particular,

$$\lim_{j\to\infty} \mu_j(B) = \mu(B) \tag{3.57}$$

holds for every μ-boundaryless Borel set B.

As usual, finite signed Radon measures are viewed as differences of finite positive Radon measures in the following.

Next, we slightly strengthen our assumptions a bit.

Hypothesis 3.9. *In addition to Hypothesis 3.1 we now assume the following conditions.*

(vii) *Suppose that V_1, and V_2 are closed operators in $\mathcal{H}$, and for each $j \in \mathbb{N}$, assume that $V_{1,j}$, and $V_{2,j}$ are closed operators in $\mathcal{H}_j$ such that*

$$\operatorname{dom}(V_1) \cap \operatorname{dom}(V_2) \supseteq \operatorname{dom}(|H_0|^{1/2}), \tag{3.58}$$

$$\operatorname{dom}(V_{1,j}) \cap \operatorname{dom}(V_{2,j}) \supseteq \operatorname{dom}(|H_{0,j}|^{1/2}), \quad j \in \mathbb{N}, \tag{3.59}$$

and

$$V = V_1^* V_2 \text{ is a self-adjoint operator in } \mathcal{H}, \tag{3.60}$$

and for each $j \in \mathbb{N}$,

$$V_j = V_{1,j}^* V_{2,j} \text{ is a self-adjoint operator in } \mathcal{H}_j. \tag{3.61}$$

(viii) *Decomposing V, V_j, $j \in \mathbb{N}$, into their positive and negative parts,*

$$\begin{aligned} V_\pm &= (1/2)[|V| \pm V], \\ V_{j,\pm} &= (1/2)[|V_j| \pm V_j], \quad j \in \mathbb{N}, \end{aligned} \tag{3.62}$$

$V_\pm$ are assumed to be infinitesimally form bounded with respect to H_0, and for each $j \in \mathbb{N}$, $V_{j,\pm}$ are assumed to be infinitesimally form bounded with respect to $H_{0,j}$.

Hypothesis 3.9 permits us to identify H and H_j with the form sums,

$$\begin{aligned} H &= H_0 +_q V, \\ H_j &= H_{0,j} +_q V_j, \quad j \in \mathbb{N}. \end{aligned} \tag{3.63}$$

It also permits one to introduce the positive and negative parts of V and V_j step by step, and in either order, that is,

$$H = (H_0 +_q V_+) +_q (-V_-) = H_0 +_q V_+ -_q V_-, \tag{3.64}$$

$$H_j = (H_{0,j} +_q V_{j,+}) +_q (-V_{j,-}) = H_{0,j} +_q V_{j,+} -_q V_{j,-}, \quad j \in \mathbb{N}, \tag{3.65}$$

with resolvent equations of the type (3.14) and (3.15) valid in each case (replacing H_0, $H_{0,j}$ by $H_0 +_q V_+$, $H_{0,j} +_q V_{j,+}$, etc.).

In this context we now decompose

$$\begin{aligned} \xi(\cdot) &= \xi(\cdot; H, H_0) \\ &= \xi(\cdot; H_0 +_q V_+ -_q V_-, H_0) \\ &= \xi(\cdot; H_0 +_q V_+ -_q V_-, H_0 +_q V_+) + \xi(\cdot; H_0 +_q V_+, H_0), \\ &= \xi_+(\cdot) - \xi_-(\cdot), \end{aligned} \tag{3.66}$$

and

$$\begin{aligned}\xi_j(\cdot) &= \xi(\cdot; H_j, H_{0,j}) \\ &= \xi(\cdot; H_{0,j} +_q V_{j,+} -_q V_{j,-}, H_{0,j}) \\ &= \xi(\cdot; H_{0,j} +_q V_{j,+} -_q V_{j,-}, H_{0,j} +_q V_{j,+}) \\ &\quad + \xi(\cdot; H_{0,j} +_q V_{+,j}, H_{0,j}) \\ &= \xi_{j,+}(\cdot) - \xi_{j,-}(\cdot),\end{aligned} \tag{3.67}$$

with $j \in \mathbb{N}$, where

$$\xi_+(\cdot) = \xi(\cdot; H_0 +_q V_+, H_0) \geq 0, \tag{3.68}$$

$$\xi_-(\cdot) = -\xi(\cdot; H_0 +_q V_+ -_q V_-, H_0 +_q V_+) \geq 0, \tag{3.69}$$

$$\xi_{j,+}(\cdot) = \xi(\cdot; H_{0,j} +_q V_{+,j}, H_{0,j}) \geq 0, \quad j \in \mathbb{N}, \tag{3.70}$$

$$\xi_{j,-}(\cdot) = -\xi(\cdot; H_{0,j} +_q V_{j,+} -_q V_{j,-}, H_{0,j} +_q V_{j,+}) \geq 0, \quad j \in \mathbb{N}. \tag{3.71}$$

Theorem 3.10. *Assume Hypothesis 3.9 and $g \in C_\infty(\mathbb{R})$. Then*

$$\lim_{j\to\infty} \int_{\mathbb{R}} \frac{\xi_j(\lambda) d\lambda}{\lambda^2+1} g(\lambda) = \int_{\mathbb{R}} \frac{\xi(\lambda) d\lambda}{\lambda^2+1} g(\lambda). \tag{3.72}$$

Proof. The basic idea of proof consists of verifying that

$$\begin{aligned}&\lim_{j\to\infty} \int_{\mathbb{R}} \frac{\xi_{j,\pm}(\lambda) d\lambda}{\lambda^2+1} P((\lambda+i)^{-1}, (\lambda-i)^{-1}) \\ &\quad = \int_{\mathbb{R}} \frac{\xi_{\pm}(\lambda) d\lambda}{\lambda^2+1} P((\lambda+i)^{-1}, (\lambda-i)^{-1})\end{aligned} \tag{3.73}$$

for all polynomials $P(\cdot,\cdot)$ in two variables, and then rely on the Stone–Weierstrass approximation in Lemma 3.5 to get

$$\lim_{j\to\infty} \int_{\mathbb{R}} \frac{\xi_{j,\pm}(\lambda) d\lambda}{\lambda^2+1} g(\lambda) = \int_{\mathbb{R}} \frac{\xi_{\pm}(\lambda) d\lambda}{\lambda^2+1} g(\lambda), \quad g \in C_\infty(\mathbb{R}), \tag{3.74}$$

and hence (3.72). To prove (3.73), it suffices to verify

$$\begin{aligned}&\lim_{j\to\infty} \int_{\mathbb{R}} \frac{\xi_{j,\pm}(\lambda) d\lambda}{\lambda^2+1} \frac{1}{(\lambda+i)^m (\lambda-i)^n} \\ &\quad = \int_{\mathbb{R}} \frac{\xi_{\pm}(\lambda) d\lambda}{\lambda^2+1} \frac{1}{(\lambda+i)^m (\lambda-i)^n},\end{aligned} \tag{3.75}$$

for $m, n \in \mathbb{N} \cup \{0\}$, which, in turn, follows once one proves

$$\lim_{j\to\infty} \int_{\mathbb{R}} \frac{\xi_{j,\pm}(\lambda) d\lambda}{\lambda^2+1} \frac{1}{(\lambda \pm i)^n} = \int_{\mathbb{R}} \frac{\xi_{\pm}(\lambda) d\lambda}{\lambda^2+1} \frac{1}{(\lambda \pm i)^n}, \quad n \in \mathbb{N} \cup \{0\}, \tag{3.76}$$

since

$$\frac{1}{(\lambda+i)^m(\lambda-i)^n} = \sum_{j=1}^{m} \frac{c_j}{(\lambda+i)^j} + \sum_{j=1}^{n} \frac{\hat{c}_j}{(\lambda-i)^j} \tag{3.77}$$

for appropriate sets of constants c_j and $\hat{c}_j$. Choosing $z = \pm i$ and $a = \mp i$ in (3.25) yields (3.76), and therefore (3.73) for all polynomials P. At this point, (3.72) follows from Lemma 3.5 once one shows the existence of an $M > 0$ for which

$$\int_{\mathbb{R}} \frac{\xi_{j,\pm}(\lambda)d\lambda}{\lambda^2+1} \leqslant M \tag{3.78}$$

for j sufficiently large. Taking (3.76) with $n = 0$, yields the convergence

$$\lim_{j\to\infty} \int_{\mathbb{R}} \frac{\xi_{j,\pm}(\lambda)d\lambda}{\lambda^2+1} = \int_{\mathbb{R}} \frac{\xi_{\pm}(\lambda)d\lambda}{\lambda^2+1}. \tag{3.79}$$

As a result, $\int_{\mathbb{R}} (1+\lambda^2)^{-1} \xi_{j,\pm}(\lambda)\, d\lambda$ is uniformly bounded with respect to $j \in \mathbb{N}$. □

An immediate consequence of Theorem 3.10 is the following vague convergence result.

Corollary 3.11. *Assume Hypothesis 3.9 and let $g \in C_0(\mathbb{R})$. Then*

$$\lim_{j\to\infty} \int_{\mathbb{R}} \xi_j(\lambda)d\lambda\, g(\lambda) = \int_{\mathbb{R}} \xi(\lambda)d\lambda\, g(\lambda). \tag{3.80}$$

Remark 3.12. If the operators $H_{0,j}$ and H_j are actually uniformly bounded from below with respect to $j \in \mathbb{N}$, and hence according to our convention (2.11), ξ and ξ_j, $j \in \mathbb{N}$, are chosen to be zero in a fixed (i.e., j-independent) neighborhood of $-\infty$, then no condition need be imposed on g in a neighborhood of $-\infty$ in (3.72) and (3.80) (apart from measurability of g, of course).

Given the decomposition (3.66)–(3.71), and introducing the measures

$$\begin{aligned} \eta_{\xi_\pm}(A) &= \int_A \frac{\xi_{\pm}(\lambda)d\lambda}{\lambda^2+1}, \\ \eta_{\xi_{j,\pm}}(A) &= \int_A \frac{\xi_{j,\pm}(\lambda)d\lambda}{\lambda^2+1}, \quad j \in \mathbb{N}, \end{aligned} \tag{3.81}$$

for $A \subseteq \mathbb{R}$ Lebesgue measurable, we are now ready for the principal result of this paper.

Theorem 3.13. *Assume Hypothesis 3.9. Then*

$$\begin{aligned} &\lim_{j\to\infty} \int_{\mathbb{R}} \frac{\xi(\lambda; H_j, H_{0,j})d\lambda}{\lambda^2+1} f(\lambda) \\ &\quad = \int_{\mathbb{R}} \frac{\xi(\lambda; H, H_0)d\lambda}{\lambda^2+1} f(\lambda), \quad f \in C_b(\mathbb{R}). \end{aligned} \tag{3.82}$$

Moreover, (3.82) *holds for every bounded Borel measurable function* f *that is* η_{ξ_+} *and* η_{ξ_-}*-almost everywhere continuous on* $\mathbb{R}$*. In particular,*

$$\lim_{j\to\infty} \int_S \frac{\xi(\lambda; H_j, H_{0,j})d\lambda}{\lambda^2+1} = \int_S \frac{\xi(\lambda; H, H_0)d\lambda}{\lambda^2+1} \tag{3.83}$$

for every set S *whose boundary has* η_{ξ_+} *and* η_{ξ_-}*-measure equal to zero.*

Proof. Again we decompose ξ and ξ_j, $j \in \mathbb{N}$, as in (3.66)–(3.71). By (3.74) and Corollary 3.11, the measure $\eta_{\xi_{j,\pm}}$ vaguely converges to the measure $\eta_{\xi_\pm}$ as $j \to \infty$, respectively. Moreover, by (3.75),

$$\lim_{j\to\infty} \eta_{\xi_{j,\pm}}(\mathbb{R}) = \eta_{\xi_\pm}(\mathbb{R}). \tag{3.84}$$

Thus, by Theorem 3.7, one concludes weak convergence of the sequence of measures $\eta_{\xi_{j,\pm}}$ to the measure $\eta_{\xi_\pm}$ as $j \to \infty$. That (3.82) holds for every bounded Borel measurable function that is $\eta_{\xi_\pm}$-almost everywhere continuous on $\mathbb{R}$ now follows directly from Theorem 3.8. Finally, convergence in (3.83) is also a direct consequence of Theorem 3.8. □

As immediate consequences of Theorem 3.13, we have the following two results.

Corollary 3.14. *Assume Hypothesis* 3.9*. Then convergence in* (3.82) *holds for any bounded Borel measurable function that is continuous almost everywhere with respect to Lebesgue measure on* $\mathbb{R}$*. In particular,* (3.83) *holds for any set* S *that is boundaryless with respect to Lebesgue measure* (*i.e., any set* S *for which the boundary of* S *has Lebesgue measure equal to zero*).

Proof. Noting that $\eta_{\xi_\pm}$ are absolutely continuous with respect to Lebesgue measure, the statements follow directly from Theorem 3.13. □

Corollary 3.15. *Assume Hypothesis* 3.9*. If* g *is a bounded Borel measurable function that is compactly supported and Lebesgue almost everywhere continuous on* $\mathbb{R}$*, then*

$$\lim_{j\to\infty} \int_{\mathbb{R}} \xi(\lambda; H_j, H_{0,j})d\lambda\, g(\lambda) = \int_{\mathbb{R}} \xi(\lambda; H, H_0)d\lambda\, g(\lambda). \tag{3.85}$$

Proof. If g satisfies the hypotheses of Corollary 3.15, then choosing

$$f(\lambda) = (\lambda^2+1)g(\lambda)$$

in (3.82) yields the result, noting that f is a bounded (g has compact support) Borel measurable function and is continuous Lebesgue-almost everywhere (and thus $\eta_{\xi_\pm}$-almost everywhere) on $\mathbb{R}$. □

Remark 3.16. We briefly summarize the instrumental role of convergence of the determinants, (3.27), in this work. The proof of (3.25) in Lemma 3.4 goes by simple induction on $n \in \mathbb{N}$ in (3.44), and it is precisely (3.27) that yields the first induction step, $n = 1$, in (3.44). Convergence of the determinants, (3.27), also proves indispensable in the proof of *weak* convergence of the spectral shift functions, that is, (3.82). To go from *vague* (cf. (3.72)) to *weak* (cf. (3.82)) convergence, we simply apply the abstract Theorem 3.7 together with convergence of the total masses, (3.84). However, it is (3.75), and therefore (3.27), that guarantees the requisite convergence of total masses, (3.84).

For applications to multi-dimensional Schrödinger operators we need to extend the assumptions in Hypothesis 3.9 a bit.

Hypothesis 3.17. *Suppose the assumptions made in Hypothesis* 3.9 *with the exception of the trace class assumptions* (3.4), (3.7), *and* (3.10).

(ix) *Assume that for some* (*and hence for all*) $z \in \rho(H_0)$,

$$\overline{V_2(H_0 - zI_{\mathcal{H}})^{-1}V_1^*},\ \overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}})^{-1}V_{j,1}^*} \oplus 0 \in \mathcal{B}_2(\mathcal{H}), \quad j \in \mathbb{N}, \tag{3.86}$$

and that

$$\begin{aligned} &\lim_{z\downarrow-\infty} \|\overline{V_2(H_0 - zI_{\mathcal{H}})^{-1}V_1^*}\|_{\mathcal{B}_2(\mathcal{H})} = 0. \\ &\lim_{z\downarrow-\infty} \|\overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}})^{-1}V_{1,j}^*} \oplus 0\|_{\mathcal{B}_2(\mathcal{H})} = 0, \quad j \in \mathbb{N}. \end{aligned} \tag{3.87}$$

(x) *Suppose that for some* (*and hence for all*) $z \in \mathbb{C}\backslash\mathbb{R}$,

$$\lim_{j\to\infty} \|[\overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1}V_{1,j}^*} \oplus 0] - \overline{V_2(H_0 - zI_{\mathcal{H}})^{-1}V_1^*}\|_{\mathcal{B}_2(\mathcal{H})} = 0. \tag{3.88}$$

Theorem 3.18. *Assume Hypothesis* 3.17. *Then the assertions of Theorem* 3.10, *Corollary* 3.11, *Theorem* 3.13, *and Corollaries* 3.14 *and* 3.15 *hold.*

Proof. It suffices to delineate the necessary changes in the proofs due to the Hilbert–Schmidt hypotheses (3.86) and (3.87) as opposed to the trace class assumptions (3.4), (3.7), and (3.10).

With (3.21) still valid, we abbreviate the modified perturbation determinants by

$$\begin{aligned} D_2(z) &= \det_{2,\mathcal{H}}(I_{\mathcal{H}} + \overline{V_2(H_0 - zI_{\mathcal{H}})^{-1}V_1^*}), \quad z \in \rho(H) \cap \rho(H_0), \\ D_{2,j}(z) &= \det_{2,\mathcal{H}_j}(I_{\mathcal{H}_j} + \overline{V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1}V_{1,j}^*}), \\ &\qquad z \in \rho(H_j) \cap \rho(H_{0,j}),\ j \in \mathbb{N}. \end{aligned} \tag{3.89}$$

Consequently, by (2.34), for $z \in \mathbb{C}\backslash\mathbb{R}$,

$$\begin{aligned} \frac{d}{dz}\ln D_2(z) &= \int_{\mathbb{R}} \frac{\xi(\lambda)d\lambda}{(\lambda - z)^2} - \operatorname{tr}_{\mathcal{H}}((H_0 - zI_{\mathcal{H}})^{-1}V(H_0 - zI_{\mathcal{H}})^{-1}), \\ \frac{d}{dz}\ln D_{2,j}(z) &= \int_{\mathbb{R}} \frac{\xi_j(\lambda)d\lambda}{(\lambda - z)^2} - \operatorname{tr}_{\mathcal{H}_j}((H_0 - zI_{\mathcal{H}_j})^{-1}V_j(H_0 - zI_{\mathcal{H}_j})^{-1}), \end{aligned} \tag{3.90}$$

for $j \in \mathbb{N}$. In analogy to (3.28), (3.29), one then obtains ($a, z \in \mathbb{C}\backslash\mathbb{R}$)

$$\begin{aligned} &(z-a)\int_{\mathbb{R}} \frac{\xi(\lambda)d\lambda}{(\lambda - a)(\lambda - z)} \\ &\quad = (z-a)\operatorname{tr}_{\mathcal{H}}(V_2(H_0 - zI_{\mathcal{H}})^{-1}\overline{(H_0 - aI_{\mathcal{H}})^{-1}V_1^*}) + \ln\left(\frac{D_2(z)}{D_2(a)}\right), \end{aligned} \tag{3.91}$$

and

$$\begin{aligned} &(z-a)\int_{\mathbb{R}} \frac{\xi_j(\lambda)d\lambda}{(\lambda - a)(\lambda - z)} \\ &\quad = (z-a)\operatorname{tr}_{\mathcal{H}_j}(V_{2,j}(H_{0,j} - zI_{\mathcal{H}_j})^{-1}\overline{(H_{0,j} - aI_{\mathcal{H}_j})^{-1}V_{1,j}^*}) + \ln\left(\frac{D_{2,j}(z)}{D_{2,j}(a)}\right), \end{aligned} \tag{3.92}$$

for $j \in \mathbb{N}$. By (3.88),

$$\lim_{j\to\infty} D_{2,j}(z) = D_2(z), \tag{3.93}$$

and by (3.11) and (3.12),

$$\begin{aligned} &\lim_{j\to\infty} \operatorname{tr}_{\mathcal{H}_j}(V_{2,j}(H_{0,j} - z)^{-1}\overline{(H_{0,j} - a)^{-1}V_{1,j}^*}) \\ &\quad = \operatorname{tr}_{\mathcal{H}}(V_2(H_0 - zI_{\mathcal{H}})^{-1}\overline{(H_0 - aI_{\mathcal{H}})^{-1}V_1^*}). \end{aligned} \tag{3.94}$$

At this point one can follow the proof of Lemma 3.4 step by step, implying the validity of (3.43). In addition, (3.90)–(3.94) yield

$$\lim_{j\to\infty}\int_{\mathbb{R}} \frac{\xi_j(\lambda)d\lambda}{(\lambda - a)(\lambda - z)} = \int_{\mathbb{R}} \frac{\xi(\lambda)d\lambda}{(\lambda - a)(\lambda - z)}, \quad a, z \in \mathbb{C}\backslash\mathbb{R}, \tag{3.95}$$

and hence the first induction step (3.45) also holds under Hypothesis 3.17, implying the assertions in Lemma 3.4. The latter is the crucial input for the proof of Theorem 3.10 and hence for Corollary 3.11, which both extend to the current Hypothesis 3.17.

Finally, the proofs of Theorem 3.13 and Corollaries 3.14 and 3.15 extend without change under Hypothesis 3.17. □

Remark 3.19. We conclude with a brief remark on an alternative approach to convergence of spectral shift functions. In cases where a fixed Hilbert space is naturally given, an abstract convergence result of spectral shift functions in the $L^1(\mathbb{R}; (\lambda^2+1)^{-1}d\lambda)$-norm, based on trace norm convergence of resolvents, has been given in [77], Lemma 8.7.5, with a refinement in the case of semibounded self-adjoint operators in [60], Lemma 8.3. This is then applied to derive relative oscillation theory results in essential spectral gaps between different Sturm–Liouville operators in [59] and [60]. This approach differs from the one developed in this paper as in our case one cannot expect subsequences of spectral functions to converge pointwise a.e. as discussed in the paragraph following (1.1).

4. Applications to Schrödinger operators

In our final section we briefly illustrate the applicability of Theorems 3.13 and 3.18 to (multi-dimensional) Schrödinger operators.

(I) The one-dimensional case. Assuming

$$V \in L^1(\mathbb{R}; dx) \text{ real-valued}, \tag{4.1}$$

and introducing the differential expression τ by

$$\tau = -\frac{d^2}{dx^2} + V(x), \quad x \in J, \tag{4.2}$$

with $J \subseteq \mathbb{R}$ an appropriate open interval, we introduce the self-adjoint Schrödinger operator $H_{(a,b),\alpha,\beta}$ in $L^2((a,b); dx)$, with Dirichlet boundary conditions at $x = a, b$

$$\begin{aligned} &(H_{(a,b),D} f)(x) = (\tau f)(x), \quad x \in (a,b), \\ &f \in \operatorname{dom}(H_{(a,b),D}) \\ &\quad = \{g \in L^2((a,b); dx) \mid \\ &\qquad g, g' \in AC([a,b]); g(a) = g(b) = 0; \tau f \in L^2((a,b); dx)\}, \end{aligned} \tag{4.3}$$

and the self-adjoint Schrödinger operator H in $L^2(\mathbb{R}; dx)$,

$$\begin{aligned} &(Hf)(x) = (\tau f)(x), \quad x \in \mathbb{R}, \\ &f \in \operatorname{dom}(H) = \{g \in L^2(\mathbb{R}; dx) \mid g, g' \in AC_{\mathrm{loc}}(\mathbb{R}); \tau f \in L^2(\mathbb{R}; dx)\}. \end{aligned} \tag{4.4}$$

Here $AC([a,b])$ (resp., $AC_{\mathrm{loc}}(\mathbb{R})$) abbreviates the set of absolutely continuous functions on $[a,b]$ (resp., the set of locally absolutely continuous functions on $\mathbb{R}$).

In the special case where $V = 0$ a.e. on $\mathbb{R}$, the operators in (4.3) and (4.4) are denoted by $H_{0,(a,b),D}$ and H_0, respectively.

The Dirichlet Green's functions (i.e., the integral kernels of the resolvents) associated with $H_{0,(a,b),D}$ and H_0 are then given by

$$\begin{aligned} &G_{0,(a,b),D}(z,x,x') \\ &\quad = (H_{0,(a,b),D} - zI_{(a,b)})^{-1}(x,x') \\ &\quad = \frac{1}{z^{1/2}\sin(z^{1/2}(b-a))} \begin{cases} \sin(z^{1/2}(x-a))\sin(z^{1/2}(b-x')), \\ \qquad\qquad a \leqslant x \leqslant x' \leqslant b, \\ \sin(z^{1/2}(x'-a))\sin(z^{1/2}(b-x)), \\ \qquad\qquad a \leqslant x' \leqslant x \leqslant b, \end{cases} \end{aligned} \tag{4.5}$$

for all $z \in \mathbb{C}\backslash\{n^2\pi^2(b-a)^{-2}\}_{n\in\mathbb{N}}$, and

$$G_0(z,x,x') = (H_0 - zI_{\mathbb{R}})^{-1}(x,x') = \frac{i}{2z^{1/2}} e^{iz^{1/2}|x-x'|}, \quad x,x' \in \mathbb{R} \tag{4.6}$$

for all $z \in \mathbb{C}\backslash[0,\infty)$ such that $\operatorname{Im}(z^{1/2}) \geqslant 0$, respectively, where I_J denotes the identity operator in $L^2(J;dx)$ for $J \subseteq \mathbb{R}$ an interval.

Moreover, we also recall the integral kernels for the square root of resolvents (cf. [32], p. 325, and [37]),

$$\begin{aligned} R^{1/2}_{0,(a,b),D}(z,x,x') &= (H_{0,(a,b),D} - zI_{(a,b)})^{-1/2}(x,x') \\ &= \frac{1}{\pi}\int_0^\infty dt\, t^{-1/2} G_{0,(a,b),D}(z-t,x,x'), \end{aligned} \tag{4.7}$$

for all $z \in \mathbb{C}\backslash\{n^2\pi^2(b-a)^{-2}\}_{n\in\mathbb{N}}$ and $x,x' \in [a,b]$, and

$$R^{1/2}_0(z,x,x') = (H_0 - zI_{\mathbb{R}})^{-1/2}(x,x') = \pi^{-1} H_0^{(1)}(z^{1/2}|x-x'|), \tag{4.8}$$

for all $z \in \mathbb{C}\backslash[0,\infty)$ such that $\operatorname{Im}(z^{1/2}) \geqslant 0$, and $x,x' \in \mathbb{R}$, where $H_0^{(1)}(\cdot)$ denotes the Hankel function of the first kind and order zero (cf. [1], Section 9.1). Moreover, employing domain monotonicity for Dirichlet Green's functions (see, e.g., [26], Section 1.VII.6), that is,

$$0 \leqslant G_{0,(a,b),D}(-E,x,x') \leqslant G_{0,(a',b'),D}(-E,x,x') \leqslant G_0(-E,x,x'), \tag{4.9}$$

for all $x,x' \in [a,b] \subseteq [a',b']$ and $E > 0$, and inserting (4.9) into (4.7) yields

$$0 \leqslant R^{1/2}_{0,(a,b),D}(-E,x,x') \leqslant R^{1/2}_0(-E,x,x'), \quad x,x' \in [a,b],\ E > 0. \tag{4.10}$$

In fact, the upper bound in (4.9) can be made more explicit by noting

$$\begin{aligned} 0 &\leqslant G_{0,(a,b),D}(-E,x,x') \\ &= \frac{1}{2E^{1/2}} \frac{[e^{E^{1/2}(x-a)} - e^{-E^{1/2}(x-a)}][e^{E^{1/2}(b-x')} - e^{-E^{1/2}(b-x')}]}{e^{E^{1/2}(b-a)} - e^{-E^{1/2}(b-a)}} \\ &= G_0(-E,x,x') - \frac{1}{2E^{1/2}} \frac{[e^{E^{1/2}(x+x'-b-a)} - e^{E^{1/2}(a+x'-b-x)}]}{e^{E^{1/2}(b-a)} - e^{-E^{1/2}(b-a)}} \\ &\quad - \frac{1}{2E^{1/2}} \frac{[e^{E^{1/2}(b+a-x-x')} - e^{E^{1/2}(x+a-b-x')}]}{e^{E^{1/2}(b-a)} - e^{-E^{1/2}(b-a)}}, \\ &\leqslant G_0(-E,x,x'), \end{aligned} \tag{4.11}$$

for $a \leqslant x \leqslant x' \leqslant b$, and analogously for $a \leqslant x' \leqslant x \leqslant b$. (One verifies that all square brackets in (4.10) are nonnegative.) The relations in (4.11) also show that

$$\lim_{a \downarrow -\infty,\, b \uparrow \infty} G_{0,(a,b),D}(-E,x,x') = G_0(-E,x,x') \quad \text{pointwise}, \tag{4.12}$$

that is, for fixed $E < 0$ and $x, x' \in \mathbb{R}$. (The latter is easily seen to extend to all fixed $z \in \mathbb{C}\backslash\mathbb{R}$.)

Next, one factors V as

$$\begin{aligned} V(x) &= u(x)v(x), \\ v(x) &= |V(x)|^{1/2}, \\ u(x) &= v(x)\,\mathrm{sgn}(V(x)), \end{aligned} \tag{4.13}$$

for all $x \in \mathbb{R}$, and introduces

$$\begin{aligned} V_{(a,b)}(x) &= V(x)|_{(a,b)}, \\ v_{(a,b)}(x) &= v(x)|_{(a,b)}, \\ u_{(a,b)}(x) &= u(x)|_{(a,b)}, \end{aligned} \tag{4.14}$$

for all $x \in (a,b)$. Then in the notation employed in Section 3,

$$u \text{ corresponds to } V_2, \qquad v \text{ corresponds to } V_1^*, \tag{4.15}$$

$$u_{(a,b)} \text{ corresponds to } V_{2,j}, \qquad v_{(a,b)} \text{ corresponds to } V_{1,j}^*, \tag{4.16}$$

$$a \downarrow -\infty,\, b \uparrow \infty \text{ corresponds to } j \longrightarrow \infty, \text{ etc.} \tag{4.17}$$

Moreover, the estimate

$$0 \leqslant |H_0^{(1)}(x)| \leqslant C \ln\Big(\frac{ex}{1+x}\Big) \frac{e^{-x}}{2\pi x^{1/2}+1}, \quad x > 0, \tag{4.18}$$

for a suitable constant $C > 0$ (cf. [1], Section 9.6, for the proper asymptotic relations as $x \downarrow 0$ and $x \to \infty$, implying (4.18)) then readily proves that

$$u(H_0 + I_{\mathbb{R}})^{-1/2},\ u(H_0 + I_{\mathbb{R}})^{-1} \in \mathcal{B}_2(L^2(\mathbb{R}; dx)), \tag{4.19}$$

$$\begin{aligned} &\overline{u(H_0 + I_{\mathbb{R}})^{-1} v} \\ &\quad = [u(H_0 + I_{\mathbb{R}})^{-1/2}][v(H_0 + I_{\mathbb{R}})^{-1/2}]^* \in \mathcal{B}_1(L^2(\mathbb{R}; dx)), \end{aligned} \tag{4.20}$$

$$[(H + I_{\mathbb{R}})^{-1} - (H_0 + I_{\mathbb{R}})^{-1}] \in \mathcal{B}_1(L^2(\mathbb{R}; dx)). \tag{4.21}$$

At this point it is possible to verify that each item in Hypothesis 3.9 applies and hence that Theorem 3.10, Corollary 3.11, Theorem 3.13, and Corollaries 3.14 and 3.15 all hold in the context of Dirichlet boundary conditions at $x = a, b$.

The case of a half-line with $\mathbb{R}$ replaced by $[0, \infty)$ and (a, b) by $(0, R)$, $R > 0$, has been dealt with in great detail in [37] (in part, using techniques developed in [34]). In [37] also the case of all separated self-adjoint boundary conditions was discussed in depth, by invoking Krein-type resolvent equations that reduce general separated boundary conditions to the case of Dirichlet boundary conditions. This strategy also applies to all separated self-adjoint boundary conditions in the current case of $\mathbb{R}$ and (a, b); we omit further details at this point. (See also [66], Chapters 2, 3, 5, and 9, for a detailed treatment of the case $n = 1$.)

(II) The two and three dimensional case (with Dirichlet boundary conditions). Assuming

$$V \in \mathcal{R}_{2,\delta} \quad \text{for some } \delta > 0, \text{ real-valued, if } n = 2, \tag{4.22}$$

$$V \in \mathcal{R}_3 \cap L^1(\mathbb{R}^3; d^3x), \quad \text{real-valued, if } n = 3, \tag{4.23}$$

where

$$\mathcal{R}_{2,\delta} = \{V \colon \mathbb{R}^2 \to \mathbb{C}, \text{ measurable} \mid V^{1+\delta}, (1 + |\cdot|^{\delta})V \in L^1(\mathbb{R}^2; d^2x)\}, \tag{4.24}$$

$$\mathcal{R}_3 = \left\{V \colon \mathbb{R}^3 \to \mathbb{C}, \text{ measurable} \mid \int_{\mathbb{R}^6} d^3x\, d^3x'\, \frac{|V(x)||V(x')|}{|x - x'|^2} < \infty\right\}, \tag{4.25}$$

(with $\mathcal{R}_3$ the set of *Rollnik* potentials), we introduce the differential expression

$$\tau = -\Delta + V(x), \quad x \in \Omega, \tag{4.26}$$

with $\Omega \subseteq \mathbb{R}^n$, $n = 2, 3$, an appropriate open set.

Denoting by $B_R \subseteq \mathbb{R}^n$, $n = 2, 3$, the open ball of radius $R > 0$, centered at the origin, we now introduce the self-adjoint Schrödinger operator $H_{B_R,D}$ in $L^2(B_R; d^nx)$, $n = 2, 3$, with *Dirichlet* boundary conditions at ∂B_R, by

$$\begin{aligned} &(H_{B_R,D} f)(x) = (\tau f)(x), \quad x \in B_R, \\ &f \in \operatorname{dom}(H_{B_R,D}) \\ &\quad = \{g \in L^2(B_R; d^nx) \mid g \in H^1_0(B_R);\ \tau g \in L^2(B_R; d^nx)\}, \end{aligned} \tag{4.27}$$

and the self-adjoint Schrödinger operator H in $L^2(\mathbb{R}^n; d^n x)$, $n = 2, 3$, by

$$\begin{aligned} &(Hf)(x) = (\tau f)(x), \quad x \in \mathbb{R}^n, \\ &f \in \operatorname{dom}(H) \\ &\quad = \{g \in L^2(\mathbb{R}^n; d^n x) \mid g \in H^1(\mathbb{R}^n);\ \tau g \in L^2(\mathbb{R}^n; d^n x)\}. \end{aligned} \tag{4.28}$$

Here $\tau f = -\Delta f + Vf$ is interpreted in the sense of distributions (i.e., in $\mathcal{D}'(B_R)$, resp., $\mathcal{D}'(\mathbb{R}^n)$, $n = 2, 3$).

In the special case where $V = 0$ a.e. on $\mathbb{R}^n$, the operators in (4.27) and (4.28) are denoted by $H_{0,B_R,D}$ and H_0, respectively, and given by

$$\begin{aligned} &H_{0,B_R,D} = -\Delta, \\ &\operatorname{dom}(H_{0,B_R,D}) \\ &\quad = \{g \in L^2(B_R; d^n x) \mid g \in H_0^1(B_R) \cap H^2(B_R);\ -\Delta g \in L^2(B_R; d^n x)\}, \end{aligned} \tag{4.29}$$

and

$$H_0 = -\Delta, \quad \operatorname{dom}(H_0) = H^2(\mathbb{R}^n). \tag{4.30}$$

The method of images (cf. [20], p. 264) then permits one to explicitly compute the Dirichlet Green's function for the ball B_R as

$$\begin{aligned} G_{0,B_R,D}(z, x, x') &= (H_{0,B_R,D} - zI_{B_R})^{-1}(x, x') \\ &= \psi_n(z, |x - x'|) - \psi_n\left(z, \frac{|x'|}{R}\left|x - \frac{R^2}{|x'|^2}x'\right|\right), \end{aligned} \tag{4.31}$$

for all $z \in \mathbb{C}\backslash[0, \infty)$ and $x \neq x'$, $x, x' \in B_R$, where

$$\psi_n(z, r) = \begin{cases} \dfrac{i}{4} H_0^{(1)}(z^{1/2} r), & n = 2, \\ \dfrac{e^{iz^{1/2}r}}{[4\pi r]}, & n = 3, \end{cases}$$

for all $z \in \mathbb{C}\backslash[0, \infty)$, such that $\operatorname{Im}(z^{1/2}) \geqslant 0$ and $r > 0$, with $H_0^{(1)}(\cdot)$ again the Hankel function of the 1st kind and order zero. Similarly,

$$\begin{aligned} G_0(z, x, x') &= (H_0 - zI_{\mathbb{R}^n})^{-1}(x, x') \\ &= \psi_n(z, |x - x'|) \\ &= \begin{cases} \frac{i}{4} H_0^{(1)}(z^{1/2}|x - x'|), & n = 2, \\ \dfrac{e^{iz^{1/2}|x-x'|}}{[4\pi|x - x'|]}, & n = 3, \end{cases} \end{aligned} \tag{4.32}$$

for all $z \in \mathbb{C}\backslash[0,\infty)$, such that $\operatorname{Im}(z^{1/2}) \geqslant 0$, with $x \neq x'$, $x, x' \in \mathbb{R}^n$, $n = 2, 3$. Here I_Ω denotes the identity operator in $L^2(\Omega; d^n x)$ for $\Omega \subseteq \mathbb{R}^n$ an open set. Consequently,

$$|G_{0,B_R,D}(z, x, x')| \leqslant C \psi_n(z, |x - x'|), \tag{4.33}$$

for all $x \neq x'$, $x, x' \in \mathbb{R}^n$, $n = 2, 3$, for some constant $C > 0$. Moreover, one gets as a pointwise limit

$$\lim_{R \to \infty} G_{0,B_R,D}(z, x, x') = G_0(z, x, x'), \tag{4.34}$$

for all $z \in \mathbb{C}\backslash[0,\infty)$, $x \neq x'$, $x, x' \in \mathbb{R}^n$.

Next, one again factors V as

$$\begin{aligned} V(x) &= u(x)v(x), \\ v(x) &= |V(x)|^{1/2}, \\ u(x) &= v(x)\,\operatorname{sgn}(V(x)), \end{aligned} \tag{4.35}$$

for all $x \in \mathbb{R}^n$, and introduces

$$\begin{aligned} V_{B_R}(x) &= V(x)|_{B_R}, \\ v_{B_R}(x) &= v(x)|_{B_R}, \\ u_{B_R}(x) &= u(x)|_{B_R}, \end{aligned} \tag{4.36}$$

for all $x \in B_R$. Then in the notation employed in Section 3,

$$u \text{ corresponds to } V_2, \qquad v \text{ corresponds to } V_1^* \tag{4.37}$$

$$u_{B_R} \text{ corresponds to } V_{2,j}, \quad v_{B_R} \text{ corresponds to } V_{1,j}^*, \tag{4.38}$$

$$B_R \longrightarrow \mathbb{R}^n \text{ as } R \uparrow \infty \text{ corresponds to } j \longrightarrow \infty, \text{ etc.}, \tag{4.39}$$

and using again the estimate (4.18) in the case $n = 2$, one concludes that for $n = 2, 3$,

$$\begin{aligned} u(H_0 + I_{\mathbb{R}^n})^{-1/2} &\in \mathcal{B}_4(L^2(\mathbb{R}^n; d^n x)), \\ u(H_0 + I_{\mathbb{R}^n})^{-1} &\in \mathcal{B}_2(L^2(\mathbb{R}^n; d^n x)), \end{aligned} \tag{4.40}$$

$$\begin{aligned} &\overline{u(H_0 + I_{\mathbb{R}^n})^{-1} v} \\ &\quad = [u(H_0 + I_{\mathbb{R}^n})^{-1/2}][v(H_0 + I_{\mathbb{R}^n})^{-1/2}]^* \in \mathcal{B}_2(L^2(\mathbb{R}^n; d^n x)), \end{aligned} \tag{4.41}$$

$$[(H + I_{\mathbb{R}^n})^{-1} - (H_0 + I_{\mathbb{R}^n})^{-1}] \in \mathcal{B}_1(L^2(\mathbb{R}^n; d^n x)), \tag{4.42}$$

$$\begin{aligned} &\overline{(H_0 + I_{\mathbb{R}^n})^{-1} V (H_0 + I_{\mathbb{R}^n})^{-1}} \\ &\quad = [u(H_0 + I_{\mathbb{R}^n})^{-1}]^* [v(H_0 + I_{\mathbb{R}^n})^{-1}] \in \mathcal{B}_1(L^2(\mathbb{R}^n; d^n x)). \end{aligned} \tag{4.43}$$

More precisely, the fact that $u(H_0 + I_{\mathbb{R}^n})^{-1} \in \mathcal{B}_2(L^2(\mathbb{R}^n; d^n x))$ follows from an application of [74], Theorem 4.1, and thus $u(H_0 + I_{\mathbb{R}^n})^{-1/2} \in \mathcal{B}_4(L^2(\mathbb{R}^n; d^n x))$ follows from the fact that $T \in \mathcal{B}_4(\mathcal{H})$ if and only if $T^*T \in \mathcal{B}_2(\mathcal{H})$. Indeed, one chooses for T the operator $u(H_0 + I_{\mathbb{R}^n})^{-1/2}$ and defines the self-adjoint and unitary operator S of multiplication by $\operatorname{sgn}(V(x))$ with $\operatorname{sgn}(V(x)) = 1$ for $V(x) \geqslant 0$ a.e. and $\operatorname{sgn}(V(x)) = -1$ for $V(x) < 0$ a.e.

Moreover, an application of [74], Proposition 4.4, then also proves that

$$\begin{aligned} &u(H_0 + I_{\mathbb{R}^n})^{-1/2} \notin \mathcal{B}_2(L^2(\mathbb{R}^n; d^n x)), \\ &\overline{u(H_0 + I_{\mathbb{R}^n})^{-1} v} \notin \mathcal{B}_1(L^2(\mathbb{R}^n; d^n x)), \end{aligned} \tag{4.44}$$

for $n = 2, 3$. Indeed, since $T^*T \in \mathcal{B}_1(\mathcal{H})$ if and only if $T \in \mathcal{B}_2(\mathcal{H})$, again choosing for T the operator $u(H_0 + I_{\mathbb{R}^n})^{-1/2}$ proves that $u(H_0 + I_{\mathbb{R}^n})^{-1/2} \notin \mathcal{B}_2(L^2(\mathbb{R}; d^n x))$ since $(|p|^2 + 1)^{-1} \notin L^2(\mathbb{R}; d^n p)$ for $n = 2, 3$.

This illustrates that even though (4.43) holds in dimensions $n = 2, 3$ (just like it holds for $n = 1$, cf. (4.21)), the use of the 2-modified Fredholm determinant $\det_{2, L^2(\mathbb{R}^n; d^n x)}(\cdot)$ in connection with formulas of the type (3.90) is inevitable in dimensions $n = 2, 3$ (as opposed to the case $n = 1$). Thus, Hypothesis 3.9 needed to be extended to Hypothesis 3.17 in order to be able to handle the multi-dimensional cases $n = 2, 3$.

We also note in connection with (2.26) that

$$\begin{aligned} \eta'(z) &= \operatorname{tr}_{L^2(\mathbb{R}^n; d^n x)}\big(\overline{(H_0 - z I_{\mathbb{R}^n})^{-1} V (H_0 - z I_{\mathbb{R}^n})^{-1}}\big) \\ &= \begin{cases} -\dfrac{1}{4\pi z} \displaystyle\int_{\mathbb{R}^2} d^2 x\, V(x), & n = 2, \\ \dfrac{i}{8\pi z^{1/2}} \displaystyle\int_{\mathbb{R}^3} d^3 x V(x), & n = 3, \end{cases} \end{aligned} \tag{4.45}$$

and hence (cf. also [33]),

$$\begin{aligned} \xi(\lambda; H, H_0) = \frac{1}{\pi} \operatorname{Im}\big(\ln\big(\det_{2, L^2(\mathbb{R}^n; d^n x)}\big(I_{\mathbb{R}^n} + \overline{u(H_0 - (\lambda + i0) I_{\mathbb{R}^n})^{-1} v}\big)\big)\big) \\ + \begin{cases} \dfrac{1}{4\pi} \displaystyle\int_{\mathbb{R}^2} d^2 x\, V(x), & \lambda > 0,\ n = 2, \\ \dfrac{\lambda^{1/2}}{4\pi^2} \displaystyle\int_{\mathbb{R}^3} d^3 x\, V(x), & \lambda > 0,\ n = 3, \\ 0, & \lambda < 0,\ n = 2, 3, \end{cases} \end{aligned} \tag{4.46}$$

in accordance with the normalization (2.11).

At this point it is possible to verify that each item in Hypothesis 3.17 applies and hence that Theorem 3.10, Corollary 3.11, Theorem 3.13, and Corollaries 3.14 and 3.15 all hold in the context of Dirichlet boundary conditions at ∂B_R for $n = 2, 3$. (We also refer to [12], [16], and the references cited therein, in the case $n = 2$, and to the detailed treatment of the case $n = 3$ in [67], Chapters I–IV.)

(iii) Possible generalizations. Without providing full details, we will hint at various possible extensions including more general regions and other boundary conditions.

In this context we find it convenient to recall some facts on positivity preserving (resp., improving) operators. Suppose $(X, \mathcal{A}, \mu)$ is a σ-finite measure space and $\mathcal{K} = L^2(X; d\mu)$ a complex, separable Hilbert space. Then $A \in \mathcal{B}(\mathcal{K})$ is called *positivity preserving* (resp., *positivity improving*) if

$$0 \neq f \in \mathcal{K},\ f \geqslant 0\ \mu\text{-a.e.} \implies Af \geqslant 0\ (\text{resp., } Af > 0)\ \mu\text{-a.e.} \tag{4.47}$$

(We refer, e.g., to [15], [21], [22], Chapter 7, [28], [29, Sect. 8], [30], [39], [42], [53], [57], [58], [61], [63], [65], Section XIII.12, [68], [70], [72], and the references cited therein for the basics of this subject.) Positivity preserving (resp., improving) of A will be denoted by

$$A \succcurlyeq 0 \quad (\text{resp., } A \succ 0). \tag{4.48}$$

(or by $0 \preccurlyeq A$ (resp., $0 \prec A$)). Similarly, if $A, B \in \mathcal{B}(\mathcal{K})$, then

$$A \succcurlyeq B \succcurlyeq 0 \quad (\text{resp., } A \succ B \succ 0) \tag{4.49}$$

(or $0 \preccurlyeq B \preccurlyeq A$ (resp., $0 \prec B \prec A$)) imply that A, B, and $A - B$ are positivity preserving (resp., positivity improving).

Considering the contraction semigroup $T(t) = e^{-tH}$, $t \geqslant 0$, with $H \geqslant 0$ self-adjoint in $\mathcal{K}$, one uses well-known relations

$$(H + \lambda I_{\mathcal{K}})^{-1} = \int_0^\infty dt\, e^{-t\lambda} e^{-tH}, \quad \lambda > 0, \tag{4.50}$$

$$e^{-tH} = \operatorname*{s-lim}_{n\to\infty} [(t/n)H + I_{\mathcal{K}}]^{-n}, \quad t \geqslant 0, \tag{4.51}$$

to prove that

$$\begin{aligned} &e^{-tH} \text{ is positivity preserving for all } t \geqslant 0 \\ \iff\ &(H + \lambda I_{\mathcal{K}})^{-1} \text{ is positivity preserving for all } \lambda > 0. \end{aligned} \tag{4.52}$$

Analogous statements hold if $H \geqslant 0$ is replaced by $H \geqslant c I_{\mathcal{K}}$ for some $c \in \mathbb{R}$.

Moreover, we note that if A is an integral operator with integral kernel $A(x, x')$ for $d\mu \otimes d\mu$-a.e. $x, x' \in X$, and assuming $A(\cdot, \cdot) \in L^1(X \times X; d\mu \otimes d\mu)$, then

$$A \succcurlyeq 0 \iff A(x, x') \geqslant 0 \text{ for } d\mu \otimes d\mu\text{-a.e. } x, x' \in X, \tag{4.53}$$

with $d\mu \otimes d\mu$ denoting the product measure on $X \times X$. Clearly, $A \succ 0$ if $A(\cdot,\cdot) > 0$ $d\mu \otimes d\mu$-a.e.

We also remark that these notions of positivity preserving (resp., improving) naturally extend to a two-Hilbert space setting in which one deals with a second Hilbert space $L^2(Y; d\nu)$ with $Y \subset X$ and $\tilde{\mu} = \mu|_Y$, see, for instance, [15], [53]. This is also frequently done in connection with (nondensely defined) quadratic forms (cf., e.g., [24], p. 61–62), and we will employ this notation in the following without further comment.

First, we turn to the case of Dirichlet boundary conditions for general nonempty, open, bounded sets $\Omega \subset \mathbb{R}^n$, $n \in \mathbb{N}$, rather than just balls $B_R \subset \mathbb{R}^n$, $R > 0$. In this context one recalls that the Dirichlet Laplacian $-\Delta_{\Omega,D}$ in $L^2(\Omega; d^n x)$, by definition, is the uniquely associated self-adjoint and strictly positive operator with the closure of the sesquilinear form

$$\int_\Omega d^n x\, \overline{(\nabla u)(x)} \cdot (\nabla v)(x), \quad f, g \in C_0^\infty(\Omega), \tag{4.54}$$

with domain the Sobolev space $H_0^1(\Omega)$ (see, e.g., [24], Section 1.8, [27], Chapter VII, [65], Section XIII.15). Domain monotonicity for the Dirichlet Laplacian then takes on the form (cf., [9], [24], Section 2.1, [65], Appendix 1 to Section XIII.12)

$$0 \preccurlyeq e^{-t(-\Delta_{\Omega_1,D})} \preccurlyeq e^{-t(-\Delta_{\Omega_2,D})}, \quad t \geqslant 0, \tag{4.55}$$

or equivalently,

$$0 \preccurlyeq (-\Delta_{\Omega_1,D} + \lambda I_{\Omega_1})^{-1} \preccurlyeq (-\Delta_{\Omega_2,D} + \lambda I_{\Omega_2})^{-1}, \quad \lambda > 0, \tag{4.56}$$

assuming $\Omega_1 \subseteq \Omega_2 \subset \mathbb{R}^n$, Ω_j nonempty, open, and bounded, $j = 1, 2$. (Positivity preserving in (4.55) and (4.56) actually extends to positivity improving if Ω_j are connected, $j = 1, 2$, and Ω_1 is strictly contained in Ω_2 such that $-\Delta_{\Omega_1,D} \neq -\Delta_{\Omega_2,D}$, cf. [53]). In particular, this yields the domain monotonicity of heat kernels,

$$0 \leqslant e^{-t(-\Delta_{\Omega_1,D})}(x,x') \leqslant e^{-t(-\Delta_{\Omega_2,D})}(x,x'), \quad t \geqslant 0,\ x, x' \in \Omega_1 \subseteq \Omega_2, \tag{4.57}$$

or equivalently, the domain monotonicity of Green's functions for Dirichlet Laplacians,

$$0 \leqslant G_{0,\Omega_1,D}(-\lambda, x, x') \leqslant G_{0,\Omega_2,D}(-\lambda, x, x'), \tag{4.58}$$

for all $\lambda > 0$, $x, x' \in \Omega_1 \subseteq \Omega_2$, $x \neq x'$, where

$$G_{0,\Omega,D}(z, x, x') = (-\Delta_{\Omega,D} - z I_\Omega)^{-1}(x, x'),$$

for all $x, x' \in \Omega$, denotes the Green's function of (i.e., the integral kernel of the resolvent of) the Dirichlet Laplacian $-\Delta_{\Omega,D}$ in $L^2(\Omega; d^n x)$, $n \in \mathbb{N}$. We note that domain monotonicity of heat kernels as in (4.57) also follows from their representation in terms of Wiener measure (see, e.g., [30], [71]).

Gaussian upper and lower bounds on heat kernels have been studied very extensively in the literature (see, e.g., [4], [23], [24], Chapter 3, [76], and the references therein). Here we just mention the rough Green's function estimate based on domain monotonicity, that is, on $\Omega \subset \mathbb{R}^n$ (see also [51], Section 1.2, [76]),

$$\begin{aligned} &G_{0,\Omega,D}(-\lambda, x, x') \\ &\quad \leqslant G_0(-\lambda, x, x') = \frac{1}{2\pi}\Big(\frac{2\pi|x-x'|}{\lambda^{1/2}}\Big)^{(2-n)/2} K_{(n-2)/2}(\lambda^{1/2}|x-x'|) \\ &\quad \leqslant \begin{cases} C_{\lambda,\Omega,n}|x-x'|^{2-n}, & n \geqslant 3, \\ C_{\lambda,\Omega}|\ln(1+|x-x'|^{-1})|, & n = 2, \end{cases} \end{aligned} \tag{4.59}$$

with $\lambda > 0$, and $x, x' \in \Omega$, $x \neq x'$, with $K_\alpha(\cdot)$ the modified irregular Bessel function of order α (cf. [1], Section 9.6) and

$$G_0(z, x, x') = (H_0 - zI_{\mathbb{R}^n})^{-1}(x, x'), \tag{4.60}$$

for all $z \in \mathbb{C}\backslash[0, \infty)$, $x, x' \in \mathbb{R}^n$, $x \neq x'$, and $n \in \mathbb{N}$, the Green's function of the self-adjoint realization of $-\Delta$ in $L^2(\mathbb{R}^n; d^n x)$,

$$H_0 = -\Delta, \quad \operatorname{dom}(H_0) = H^2(\mathbb{R}^n). \tag{4.61}$$

The estimate (4.59) ignores all effects of the boundary $\partial\Omega$ of Ω, but it suffices for the purpose at hand (cf. (4.18) and (4.32)).

It is worth noting that these considerations extend to Schrödinger operators defined as form sums $-\Delta_{\Omega,D} +_q V$ in $L^2(\Omega; d^n x)$, assuming $0 \leqslant V \in L^1_{\mathrm{loc}}(\Omega; d^n x)$, $n \in \mathbb{N}$ (and also to additional, appropriately relatively form bounded, potentials), see [24], Chapters 1–3. In addition, a Feynman–Kac approach to semigroups can be applied as long as $V_\pm$ belong to appropriate Kato classes (cf. [2], [17], and [25]).

The case of Neumann boundary conditions, and more generally, that of Robin boundary conditions, is a bit more involved as domain monotonicity does not hold even for general convex domains (cf. [7] and [46]) and a certain regularity of the boundary $\partial\Omega$ of Ω needs to be assumed. In addition, reflecting Brownian motion only works for special and sufficiently regular domains $\Omega \subset \mathbb{R}^n$. Still, one can proceed along the following lines, assuming Ω to be bounded and smooth, for simplicity. (The case of minimally smooth, that is, bounded Lipschitz domains, will be considered elsewhere [36].)

The Neumann sesquilinear form in $L^2(\Omega; d^n x)$ is given by

$$\int_\Omega d^n x\, \overline{(\nabla u)(x)} \cdot (\nabla v)(x), \quad u, v \in H^1(\Omega), \tag{4.62}$$

and its uniquely associated self-adjoint and nonnegative operator in $L^2(\Omega; d^n x)$ represents the Neumann Laplacian $-\Delta_{\Omega,N}$. The corresponding Neumann boundary

condition then reads $(\partial u/\partial \nu)|_{\partial\Omega} = 0$, $u \in \operatorname{dom}(-\Delta_{\Omega,N})$, with ν the normal unit vector to $\partial\Omega$ and $\partial/\partial\nu$ denoting the normal derivative.

Similarly, for $\theta \in C(\partial\Omega)$, the Robin sesquilinear form is of the type

$$\int_\Omega d^n x\, \overline{(\nabla u)(x)} \cdot (\nabla v)(x) + \int_{\partial\Omega} d^{n-1}\omega(\xi)\, \theta(\xi)\overline{u(\xi)}v(\xi), \quad u, v \in H^1(\Omega), \tag{4.63}$$

with $d^{n-1}\omega$ the surface measure on $\partial\Omega$ (cf. [35] for more details). The uniquely associated self-adjoint operator in $L^2(\Omega; d^n x)$ then represents the Robin Laplacian $-\Delta_{\Omega,\theta}$. The corresponding Robin boundary condition is of the form $(\partial u/\partial\nu)|_{\partial\Omega} + \theta\, u|_{\partial\Omega} = 0$, $u \in \operatorname{dom}(-\Delta_{\Omega,\theta})$.

Assuming $\Omega_1 \subseteq \Omega_2$ and $0 \leqslant \theta_1(\xi) \leqslant \theta_2(\xi)$, $\xi \in \partial\Omega_2$ one then has the positivity preserving relations proved in [15], [53] (see also [10], p. 22)

$$\begin{aligned} 0 &\leqslant e^{-t(-\Delta_{\Omega_1,D})} \leqslant e^{-t(-\Delta_{\Omega_2,D})} \\ &\leqslant e^{-t(-\Delta_{\Omega_2,\theta_2})} \leqslant e^{-t(-\Delta_{\Omega_2,\theta_1})} \leqslant e^{-t(-\Delta_{\Omega_2,N})}, \end{aligned} \tag{4.64}$$

for $t \geqslant 0$, or, equivalently,

$$\begin{aligned} 0 &\leqslant (-\Delta_{\Omega_1,D} + \lambda I_{\Omega_1})^{-1} \leqslant (-\Delta_{\Omega_2,D} + \lambda I_{\Omega_2})^{-1} \\ &\leqslant (-\Delta_{\Omega_2,\theta_2} + \lambda I_{\Omega_2})^{-1} \leqslant (-\Delta_{\Omega_2,\theta_1} + \lambda I_{\Omega_2})^{-1} \\ &\leqslant (-\Delta_{\Omega_2,N} + \lambda I_{\Omega_2})^{-1}, \end{aligned} \tag{4.65}$$

for $\lambda > 0$. (Again, positivity preserving in (4.64) and (4.65) actually extends to positivity improving if Ω_j are connected, $j = 1, 2$, Ω_1 is strictly contained in Ω_2 such that $-\Delta_{\Omega_1,D} \neq -\Delta_{\Omega_2,D}$, and $\theta_1 \neq \theta_2$ such that $-\Delta_{\Omega_2,\theta_1} \neq -\Delta_{\Omega_2,\theta_2}$, cf. [53]).

Relations (4.64) and (4.65) then yield analogous pointwise bounds on heat kernels and Green's functions to those in (4.57) and (4.58) and we note that Gaussian upper bounds for Neumann heat kernels are available in the literature (see, e.g., [4] or [24], Theorem 3.2.9).

We conclude by noting that in dimensions $n \geqslant 3$, suitably higher modified Fredholm determinants $\det_{p,L^2(\mathbb{R}^n;d^n x)}(\cdot)$, $p = p(n) \in \mathbb{N}$, must be applied. This is discussed in some detail in [78] and in [79], Chapter 9, and under somewhat different assumptions on V (sign definiteness of V, but otherwise more general local singularities of V are permitted) in [54], Section 1.6. It is possible to remove the sign definiteness assumptions on V (as discussed in parts (I) and (II), see also [54], Theorem 1.61, for $1 \leqslant n \leqslant 3$). Moreover, one should establish the connection with higher-order spectral shift functions (the Koplienko spectral shift function for Hilbert–Schmidt class perturbations $\mathcal{B}_2(L^2(\mathbb{R}^n; d^n x))$ and its recent extension to $\mathcal{B}_p(L^2(\mathbb{R}^n; d^n x))$-perturbations, $p \in \mathbb{N}$, $p \geqslant 3$, derived in [64] (see also [3]). This lies beyond the scope of this paper and will be taken up elsewhere.

References

[1] M. Abramowitz and I. A. Stegun, *Handbook of mathematical functions with formulas, graphs, and mathematical tables. 10*th *printing, with corrections.* National Bureau of Standards. John Wiley & Sons, New York etc., 1972. MR 0167642 Zbl 0543.33001

[2] M. Aizenman and B. Simon, Brownian motion and Harnack inequality for Schrödinger operators. *Commun. Pure Appl. Math.* **35** (1982), 209–273. MR 0644024 Zbl 0459.60069

[3] A. B. Aleksandrov and V. V. Peller, Trace formulae for perturbations of class S_m. *J. Spectr. Theory* **1** (2011), 1–26. MR 2820884

[4] W. Arendt and A. F. M. ter Elst, Gaussian estimates for second order elliptic operators with boundary conditions. *J. Operator Theory* **38** (1997), 87–130. MR 1462017 Zbl 0879.35041

[5] N. Aronszajn and W. F. Donoghue, On exponential representations of analytic functions in the upper half-plane with positive imaginary part. *J. Analyse Math.* **5** (1957), 321–388. Zbl 0138.29502

[6] K. Asano and Y. Shizuta, On the theory of linear equations and Fredholm determinants. *Publ. Res. Inst. Math. Sci., Kyoto Univ., Ser. A* **3** (1968), 417–450. MR 0244802 Zbl 0182.17201

[7] R. F. Bass and K. Burdzy, On domain monotonicity of the Neumann heat kernel. *J. Funct. Anal.* **116** (1993), 215–224. MR 1237993 Zbl 0794.35065

[8] H. Bauer, *Measure and integration theory.* De Gruyter Studies in Mathematics **26**. Walter de Gruyter & Co., Berlin, 2001. Partial English transl. of *Wahrscheinlichkeitstheorie und Grundzüge der Maßtheorie.* Walter de Gruyter & Co., Berlin, 1968. MR 1897176 (Englinh ed.) MR 0239626 (German ed.) Zbl 0985.28001 (English ed.) Zbl 0174.48802 (German ed.)

[9] A. Ben Amor and W. Hansen, Continuity of eigenvalues for Schrödinger operators, L^p-properties of Kato type integral operators. *Math. Ann.* **321** (2001), 925–953.

[10] S. Bergmann and M. Schiffer, *Kernel functions and elliptic differential equations in mathematical physics.* Academic Press Inc., London, 1953. Reprint Dover Publications, Mineola (NY), 2005. MR 0054140 Zbl 0053.39003 Zbl 1204.35004 (reprint)

[11] M. Sh. Birman and D. R. Yafaev, The spectral shift function. The work of M. G. Krein and its further development. *St. Petersburg Math. J.* **4** (1993), 833–870. English transl. of *Algebra i Analiz* **4** (1992), 1–44. MR 1202723 Zbl 0791.47013

[12] D. Bollé, F. Gesztesy, and C. Danneels, Threshold scattering in two dimensions. *Ann. Inst. H. Poincaré, Phys Théor.* **48** (1988), 175–204. MR 0952661 Zbl 0696.35040

[13] V. Borovyk, *Box approximation and related techniques in spectral theory.* Ph.D. thesis. University of Missouri, Columbia, 2008. MR 2713679

[14] V. Borovyk and K. A. Makarov, On the weak and ergodic limit of the spectral shift function. *Lett. Math. Phys.* **100** (2012), 1–15.

[15] O. Bratteli, A. Kishimoto, and D. W. Robinson, Positivity and monotonicity properties of C_0-semigroups. I. *Commun. Math. Phys.* **75** (1980), 67–84. MR 0581570 Zbl 0453.47020

[16] M. Cheney, Two-dimensional scattering: The number of bound states from scattering data. *J. Math. Phys.* **25** (1984), 1449–1455. MR 0745757 Zbl 0554.35094

[17] K. L. Chung and Z. Zhao, *From Brownian motion to Schrödinger's equation.* Springer Verlag, Berlin, 1995. MR 1329992 Zbl 0819.60068

[18] J. M. Combes, P. D. Hislop, F. Klopp, and S. Nakamura, The Wegner estimate and the integrated density of states for some random operators. In P. D. Hislop and M. Krishna (eds.), *Spectral and inverse spectral theory. Papers from the Indo-US Workshop on Spectral and Inverse Spectral Problems for Schrödinger Operators held at the University of Goa, Goa, December 14–20, 2000.* Proc. Indian Acad. Sci. (Math. Sci.) **112**, Indian Academy of Sciences, Bangalore, 2002, 31–53. MR 1894541

[19] J. M. Combes, P. D. Hislop, and S. Nakamura, The L^p-theory of the spectral shift function, the Wegner estimate, and the integrated density of states for some random operaors. *Commun. Math. Phys.* **218** (2001), 113–130. MR 1824200 Zbl 1042.82024

[20] R. Courant and D. Hilbert, *Methods of mathematical physics, Vol.* II. Interscience Publishers (a division of John Wiley & Sons), New York, 1962. Reprint 1989. Transl. and revised from *Methoden der mathematischen Physik.* Vol II. Interscience Publishers, New York, 1943. MR 0140802 (1962) MR 1894539 (1989) MR 0009069 (German ed.) Zbl 0099.29504 (1962) Zbl 0729.35001 (1989) Zbl 0061.16602 (German ed.)

[21] E. B. Davies, Properties of the Green's functions of some Schrödinger operators. *J. London Math. Soc.,* II *Ser.* **7** (1974), 483–491. MR 0342847 Zbl 0271.47003

[22] E. B. Davies, *One-parameter semigroups.* London Mathematical Society Monographs **15**. Academic Press, A Subsidiary of Harcourt Brace Jovanovich, Publishers, London and New York, 1980. MR 0591851 Zbl 0457.47030

[23] E. B. Davies, *Explicit constants for Gaussian upper bounds on heat kernels. Amer. J. Math.* **109** (1987), 319–334. MR 0882426 Zbl 0659.35009

[24] E. B. Davies, *Heat kernels and spectral theory.* Cambridge Tracts in Mathematics **92**. Cambridge University Press, Cambridge, 1989. Softcover ed. 1990. MR 0990239 MR 1103113 (softcover ed.) Zbl 0699.35006

[25] M. Demuth and J. van Casteren, *Stochastic spectral theory for selfadjoint Feller operators. A functional integration approach.* Birkhäuser, Basel, 2000. MR 1772266 Zbl 0980.60005

[26] J. L. Doob, *Classical potential theory and its probabilistic counterpart.* Springer Verlag, New York, 1984. MR 0731258 Zbl 0549.31001

[27] D. E. Edmunds and W. D. Evans, *Spectral theory and differential operators.* Clarendon Press, Oxford, 1987. Paperback ed. 1989. MR 0929030 Zbl 0628.47017 Zbl 0664.47014 (paperback ed.)

[28] W. G. Faris, *Invariant cones and uniqueness of the ground state for Fermion systems. J. Math. Phys.* **13** (1972), 1285–1290. MR 0321451 Zbl 0245.47041

[29] W. G. Faris, *Self-adjoint operators.* Lecture Notes in Mathematics **433**. Springer Verlag, Berlin etc., 1975. MR 0467348 Zbl 0317.47016

[30] W. Faris and B. Simon, Degenerate and non-degenerate ground states for Schrödinger operators. *Duke Math. J.* **42** (1975), 559–567. MR 0381571 Zbl 0339.35033

[31] R. Geisler, V. Kostrykin, and R. Schrader, Concavity properties of Krein's spectral shift function. *Rev. Math. Phys.* **7** (1995), 161–181. MR 1317338 Zbl 0836.47049

[32] F. Gesztesy and H. Holden, *Soliton Equations and Their Algebro-Geometric Solutions. Vol.* I. $(1+1)$*-Dimensional Continuous Models.* Cambridge Studies in Advanced Mathematics **79**. Cambridge University Press, Cambridge, 2003. MR 1992536 Zbl 1061.37056

[33] F. Gesztesy, Y. Latushkin, M. Mitrea, and M. Zinchenko, Nonselfadjoint operators, infinite determinants, and some applications. *Russ. J. Math. Phys.* **12** (2005), 443–471. MR 2201310 Zbl 1201.47028

[34] F. Gesztesy and K. A. Makarov, (Modified) Fredholm determinants for operators with matrix-valued semi-separable integral kernels revisited. *Integral Equations Operator Theory* **47** (2003), 457–497. Erratum ibid. **48** (2004), 425–426. Corrected electronic only version ibid. **48** (2004), 561–602. MR 2021969 MR 2038511 (erratum) Zbl 1084.47015

[35] F. Gesztesy and M. Mitrea. Nonlocal Robin Laplacians and some remarks on a paper by Filonov on eigenvalue inequalities. *J. Differential Equations* **247** (2009), 2871–2896. MR 2568160 Zbl 1181.35155

[36] F. Gesztesy, M. Mitrea, and R. Nichols, Heat kernel bounds for elliptic partial differential operators in divergence form with Robin-type boundary conditions. In preparation.

[37] F. Gesztesy and R. Nichols, Weak Convergence of Spectral Shift Functions for One-Dimensional Schrödinger Operators. To appear in *Math. Nachr.* Preprint 2011 arXiv:1111.0095

[38] F. Gesztesy and M. Zinchenko, Symmetrized perturbation determinants and applications to boundary data maps and Krein-type resolvent formulas. *Proc. London Math. Soc.* (3) **104** (2012), 577–612. Zbl 06021281

[39] H.-W. Goelden, On non-degeneracy of the ground state of Schrödinger operators. *Math. Z.* **155** (1977), 239–247. MR 0609535 Zbl 0353.35032

[40] I. C. Gohberg and M. G. Krein, *Introduction to the theory of linear nonselfadjoint operators.* Translations of Mathematical Monographs **18**. Amer. Math. Soc., Providence (RI), 1969. MR 0246142 Zbl 0181.13504

[41] H. R. Grümm, Two theorems about $\mathfrak{C}_p$. *Rep. Math. Phys.* **4** (1973), 211–215. MR 0327208 Zbl 0258.47022

[42] H. Hess, R. Schrader, and D. A. Uhlenbrock, Domination of semigroups and generalization of Kato's inequality. *Duke Math. J.* **44** (1977), 893–904. MR 0458243 Zbl 0379.47028

[43] P. D. Hislop and F. Klopp, The integrated density of states for some random operators with nonsign definite potentials. *J. Funct. Anal.* **195** (2002), 12–47. MR 1934351 Zbl 1013.60046

[44] P. D. Hislop and P. Müller, The spectral shift function for compactly supported perturbations of Schrödinger operators on large bounded domains. *Proc. Amer. Math. Soc.* **138** (2010), 2141–2150. MR 2596053 Zbl 1190.81127

[45] P. D. Hislop and P. Müller, Uniform convergence of spectral shift functions. In N. Minami (ed.), *Papers from the RIMS Workshop held at Kyoto University, Kyoto, December 2–4, 2009.* RIMS Kôkyôroku Bessatsu **B27**. Research Institute for Mathematical Sciences (RIMS), Kyoto, 2011, 35–43. MR 2885253

[46] E. P. Hsu, A domain monotonicity property of the Neumann heat kernel. *Osaka J. Math.* **31** (1994), 215–223. MR 1262798 Zbl 0817.60074

[47] D. Hundertmark, R. Killip, S. Nakamura, P. Stollmann, and I. Veselic, Bounds on the spectral shift function and the density of states. *Commun. Math. Phys.* **262** (2006), 489–503. MR 2200269 Zbl 1121.47006

[48] D. Hundertmark and B. Simon, An optimal L^p-bound on the Krein spectral shift function. *J. Anal. Math.* **87** (2002), 199–208. MR 1945282 Zbl 1054.47020

[49] T. Hupfer, H. Leschke, P. Müller, and S. Warzel, Existence and uniqueness of the integrated density of states for Schrödinger operators with magnetic fields and unbounded random potentials. *Rev. Math. Phys.* **13** (2001), 1547–1581. MR 1869817 Zbl 1029.81027

[50] T. Kato, Wave operators and similarity for some non-selfadjoint operators. *Math. Ann.* **162** (1966), 258–279. MR 0190801 Zbl 0139.31203

[51] C. E. Kenig, Harmonic Analysis Techniques for Second Order Elliptic Boundary Value Problems. CBMS Regional Conference Series in Mathematics **83**. Amer. Math. Soc., Providence (RI), 1994. MR 1282720 Zbl 0812.35001

[52] W. Kirsch, Small perturbations and the eigenvalues of the laplacian on large bounded domains. *Proc. Amer. Math. Soc.* **101** (1987), 509–512. MR 0908658 Zbl 0643.35074

[53] A. Kishimoto and D. W. Robinson, Positivity and monotonicity properties of C_0-semigroups II. *Commun. Math. Phys.* **75** (1980), 84–101. MR 0581571 Zbl 0453.47021

[54] V. Kostrykin, *Die spektrale Shiftfunction und ihre Anwendungen auf zufällige Schrödingeroperatoren.* Habilitationsschrift, Technical University of Aachen, Aachen, 1999.

[55] V. Kostrykin and R. Schrader, Scattering theory approach to random Schrödinger operators in one dimension. *Rev. Math. Phys.* **11** (1999), 187–242. MR 1681197 Zbl 0957.60101

[56] V. Kostrykin and R. Schrader, The density of states and the spectral shift density of random Schrödinger operators. *Rev. Math. Phys.* **12** (2000), 807–847. MR 1770547 Zbl 0961.47022

[57] M. A. Krasnoselskii, *Positive solutions of operator equations.* Noordhoff, Groningen, 1964. Original Russian Gosudarstv. Izdat. Fiz.-Mat. Lit., Moscow, 1963. MR MR0181881 (English ed.) MR MR0145331 (Russian ed.) Zbl 0121.10604

[58] M. G. Krein and M. A. Rutman, Linear operators leaving invariant a cone in a Banach space. *Amer. Math. Soc. Transl.* **26** (1950). Original Russian *Uspehi Matem. Nauk* (*N. S.*) **3** (1948), 3–95. MR 0038008 (English ed.) MR 0027128 (Russian ed.) Zbl 0030.12902

[59] H. Krüger and G. Teschl, Relative oscillation theory for Sturm–Liouville operators extended. *J. Funct. Anal.* **254** (2008), 1702–1720. MR 2396019 Zbl 1144.34014

[60] H. Krüger and G. Teschl, Relative oscillation theory, weighted zeros of the Wronskian, and the spectral shift function. *Commun. Math. Phys.* **287** (2009), 613–640. MR 2481752 Zbl 1186.47009

[61] S. Miyajima and N. Okazawa, Generators of positive C_0-semigroups. *Pac. J. Math.* **125** (1986), 161–175. MR 0860756 Zbl 0615.47031

[62] S. Nakamura, A remark on the Dirichlet–Neumann decoupling and the integrated density of states. *J. Funct. Anal.* **179** (2001), 136–152. MR 1807255 Zbl 0970.35084

[63] M. A. Perelmuter, Positivity preserving operators and one criterion of essential self-adjointness. *J. Math. Anal. Appl.* **82** (1981), 406–419. MR 0629767 Zbl 0482.47017

[64] D. Potapov, A. Skripka, and F. Sukochev, Spectral shift function of higher order. Preprint 2009. arXiv:0912.3056

[65] M. Reed and B. Simon, *Methods of modern mathematical physics* IV. *Analysis of operators.* Academic Press, New York etc., 1978. MR 0493421 Zbl 0401.47001

[66] M. Schechter, *Operator methods in quantum mechanics.* North Holland Publishing Co., New York etc., 1981. Reprint Dover Publications, Mineola (NY), 2002. MR 0597895 MR 1969612 (reprint) Zbl 0456.47012 Zbl 1029.47054 (reprint)

[67] B. Simon, *Quantum mechanics for Hamiltonians defined as quadratic forms.* Princeton University Press, Princeton (NJ), 1971. MR 0455975 Zbl 0232.47053

[68] B. Simon, Ergodic semigroups of positivity preserving self-adjoint operators. *J. Funct. Anal.* **12** (1973), 335–339. MR 0358434 Zbl 0252.47034

[69] B. Simon, Notes on infinite determinants of Hilbert space operators. *Adv. Math.* **24** (1977), 244–273. MR 0482328 Zbl 0353.47008

[70] B. Simon, An abstract Kato's inequality for generators of positivity preserving semigroups. *Indiana Univ. Math. J.* **26** (1977), 1067–1073. MR 0389.47021 Zbl 0389.47021

[71] B. Simon, Classical boundary conditions as a technical tool in modern mathematical physics. *Adv. Math.* **30** (1978), 268–281. MR 0520236 Zbl 0414.35069

[72] B. Simon, Kato's inequality and the comparison of semigroups. *J. Funct. Anal.* **32** (1979), 97–101. MR 0533221 Zbl 0413.47037

[73] B. Simon, Schrödinger semigroups. Bull. Amer. Math. Soc. **7**, 447–526 (1982). MR 0670130 Zbl 0524.35002

[74] B. Simon, *Trace ideals and their applications. Second ed.* Mathematical Surveys and Monographs **120**. Amer. Math. Soc., Providence (RI), 2005. MR 2154153 Zbl 1074.47001

[75] A. V. Sobolev, Efficient bounds for the spectral shift function. *Ann. Inst. H. Poincaré, Phys. Théor.* **58** (1993), 55–83. MR 1208792 Zbl 0813.47006

[76] M. van den Berg, Gaussian bounds for the Dirichlet heat kernel. *J. Funct. Anal.* **88** (1990), 267–278. MR 1038442 Zbl 0705.35052

[77] D. R. Yafaev, *Mathematical scattering theory. General theory.* Transl. Math. Monographs **105**. Amer. Math. Soc., Providence (RI), 1992. MR 1180965 Zbl 0761.47001

[78] D. R. Yafaev, Perturbation determinants, the spectral shift function, trace identities, and all that. *Funct. Anal. Appl.* **41** (2007), 217–236. Original Russian *Funkts. Anal. Prilozh.* **41** (2007), 60–83. MR 2381955 Zbl 1222.47072

[79] D. R. Yafaev, Mathematical Scattering Theory. Analytic Theory. Mathematical Surveys and Monographs **158**. Amer. Math. Soc., Providence, (RI), 2010. MR 2598115 Zbl 1197.35006

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