Applications of Spectral Shift Functions. III: Boundary Data and Dirichlet-to-Neumann Maps

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Motivation and Some Literature:

- **Overarching Topic: Self-adjoint extensions** and **boundary data maps** (i.e., extensions of the **Dirichlet-to-Neumann map**).

- We'll treat **all self-adjoint boundary conditions** for **regular Schrödinger operators** on a **finite** interval. In particular, we'll describe the **Krein–von Neumann extension**.

- **Krein-type resolvent formulas.**

- **Trace formulas.**

- **Symmetrized (Fredholm) perturbation determinants.**

- **Krein spectral shift functions.**

Motivation and Some Literature (contd.):

S. Clark, F. G., and M. Mitrea, *Boundary Data Maps for Schrödinger Operators on a Compact Interval*, Math. Modelling Nat. Phenomena **5**, No. 4, 73–121 (2010).

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

S. Clark, F. G., R. Nichols, and M. Zinchenko, *Boundary data maps and Krein's resolvent formula for Sturm–Liouville operators on a finite interval*, Operators and Matrices **8**, 1–71 (2014).

A Bit of Notation:

- $\mathcal{H}$ denotes a (separable, complex) Hilbert space, $I_{\mathcal{H}}$ represents the identity operator in $\mathcal{H}$.
- If A is a closed (typically, self-adjoint) operator in $\mathcal{H}$, then
- $\rho(A) \subseteq \mathbb{C}$ denotes the **resolvent set** of A; $z \in \rho(A) \iff A - z\, I_{\mathcal{H}}$ is a bijection.
- $\sigma(A) = \mathbb{C} \backslash \rho(A)$ denotes the **spectrum** of A.
- $\sigma_p(A)$ denotes the **point spectrum** (i.e., the set of eigenvalues) of A.
- $\sigma_d(A)$ denotes the **discrete spectrum** of A (i.e., isolated eigenvalues of finite (algebraic) multiplicity).
- If A is closable in $\mathcal{H}$, then $\overline{A}$ denotes the **operator closure** of A in $\mathcal{H}$.

Note. All operators will be **linear** in this course.

A Bit of Notation (contd.):

- $\mathcal{B}(\mathcal{H})$ is the set of **bounded** operators defined on $\mathcal{H}$.

  $\mathcal{B}_p(\mathcal{H})$, $1 \leq p \leq \infty$ denotes the pth trace ideal of $\mathcal{B}(\mathcal{H})$,

  (i.e., $T \in \mathcal{B}_p(\mathcal{H}) \Longleftrightarrow \sum_{j \in \mathcal{J}} \lambda_j\big((T^*T)^{1/2}\big)^p < \infty$, where $\mathcal{J} \subseteq \mathbb{N}$ is an appropriate index set, and the eigenvalues $\lambda_j(T)$ of T are repeated according to their algebraic multiplicity),

  $\mathcal{B}_1(\mathcal{H})$ is the set of **trace class** operators,

  $\mathcal{B}_2(\mathcal{H})$ is the set of **Hilbert–Schmidt** operators,

  $\mathcal{B}_\infty(\mathcal{H})$ is the set of **compact** operators.

- $\operatorname{tr}_{\mathcal{H}}(A) = \sum_{j \in \mathcal{J}} \lambda_j(A)$ denotes the **trace** of $A \in \mathcal{B}_1(\mathcal{H})$.

- $\det_{\mathcal{H}}(I_{\mathcal{H}} - A) = \prod_{j \in \mathcal{J}} [1 - \lambda_j(A)]$ denotes the **Fredholm determinant**, defined for $A \in \mathcal{B}_1(\mathcal{H})$.

- $\det_{2,\mathcal{H}}(I_{\mathcal{H}} - B) = \prod_{j \in \mathcal{J}} [1 - \lambda_j(B)] e^{\lambda_j(B)}$ denotes the **modified Fredholm determinant**, defined for $B \in \mathcal{B}_2(\mathcal{H})$.

Maximal and Minimal Schrödinger Operators

Let

$$V \in L^1((0,R);dx) \text{ be } \textbf{real-valued}, \ R \in (0,\infty),$$

and introduce the Schrödinger differential expression τ via

$$\tau = -\frac{d^2}{dx^2} + V(x), \quad x \in (0,R),$$

and the associated **maximal** and **minimal** operators in $L^2((0,R);dx)$ associated with τ by

$$\begin{aligned}
&H_{\max} f = \tau f, \\
&f \in \operatorname{dom}(H_{\max}) = \big\{ g \in L^2((0,R);dx) \,\big|\, g, g' \in \mathrm{AC}([0,R]);\ \tau g \in L^2((0,R);dx) \big\}, \\
&H_{\min} f = \tau f, \\
&f \in \operatorname{dom}(H_{\min}) = \{ g \in \operatorname{dom}(H_{\max}) \,|\, g(0) = g'(0) = g(R) = g'(R) = 0 \}.
\end{aligned}$$

$\mathrm{AC}([0,R])$ denotes the set of absolutely continuous functions on $[0,R]$.

Note. Much (but not all) of this material extends to the **non-self-adjoint** case.

Self-Adjoint Extensions of $H_{\min}$

Introduce the following families of **self-adjoint** extensions H_{θ_0,θ_R} and $H_{F,\phi}$ in $L^2((0,R);dx)$ of the minimal operator $H_{\min}$,

$$\begin{aligned} &H_{\theta_0,\theta_R} f = \tau f, \quad \theta_0, \theta_R \in [0,\pi), \\ &f \in \operatorname{dom}(H_{\theta_0,\theta_R}) = \big\{ g \in \operatorname{dom}(H_{\max}) \,\big|\, \cos(\theta_0) g(0) + \sin(\theta_0) g'(0) = 0, \\ &\qquad\qquad\qquad\qquad\qquad\qquad \cos(\theta_R) g(R) - \sin(\theta_R) g'(R) = 0 \big\} \end{aligned}$$

and

$$\begin{aligned} &H_{F,\phi} f = \tau f, \quad \phi \in [0,2\pi), \ F \in \mathrm{SL}(2,\mathbb{R}), \\ &f \in \operatorname{dom}(H_{F,\phi}) = \left\{ g \in \operatorname{dom}(H_{\max}) \,\middle|\, \begin{pmatrix} g(R) \\ g'(R) \end{pmatrix} = e^{i\phi} F \begin{pmatrix} g(0) \\ g'(0) \end{pmatrix} \right\}. \end{aligned}$$

$\mathrm{SL}(2,\mathbb{R})$ denotes the set of 2×2 matrices with determinant $= 1$ and real entries.

Claim: There's nothing else that's self-adjoint!

Self-Adjoint Extensions of $H_{\min}$ contd.

Theorem 1 (Weidmann 2003 (German edition), Thm. 13.15)

H_{θ_0,θ_R} and $H_{F,\phi}$ are self-adjoint extensions of $H_{\min}$ for all $\theta_0, \theta_R \in [0,\pi)$, $\phi \in [0, 2\pi)$, and $F \in \mathrm{SL}(2,\mathbb{R})$.

Conversely, let $\widetilde{H}$ be a self-adjoint extension of $H_{\min}$. Then either $\widetilde{H} = H_{\theta_0,\theta_R}$ for some $\theta_0, \theta_R \in [0,\pi)$, or else, $\widetilde{H} = H_{F,\phi}$ for some $\phi \in [0, 2\pi)$ and $F \in \mathrm{SL}(2,\mathbb{R})$.

Note: Weidmann actually proves this for general Sturm–Liouville operators in $L^2((a,b); r(x)dx)$ generated by the **regular** differential expression

$$\tau = \frac{1}{r(x)}\left[-\frac{d}{dx}p(x)\frac{d}{dx} + q(x)\right], \quad x \in (a,b),$$

assuming the usual conditions $r > 0$ a.e. on (a,b), $r \in L^1_{\mathrm{loc}}((a,b);dx)$, $p > 0$ a.e. on (a,b), $1/p \in L^1_{\mathrm{loc}}((a,b);dx)$, $q \in L^1_{\mathrm{loc}}((a,b);dx)$, q real-valued a.e. on (a,b).

Krein's Formula: Abstract Setting

Let A be a densely defined, symmetric operator in $\mathcal{H}$ with **finite** deficiency indices (m, m). Let A_1 and A_2 denote two self-adjoint extensions of A, **relatively prime** with respect to their maximal common part A_0, that is,

$$\operatorname{dom}(A_1) \cap \operatorname{dom}(A_2) = \operatorname{dom}(A_0).$$

For a fixed $z_0 \in \rho(A_1) \cap \rho(A_2)$, let $\{g_k(z_0)\}_{k=1}^r$ be a fixed basis for $\ker(A_0^* - z_0)$ $(0 \leq r \leq m)$, and define

$$U_{z,z_0} = (A_1 - z_0)(A_1 - z)^{-1}, \quad z \in \rho(A_1).$$

Then the following hold:

$\{g_k(z)\}_{k=1}^r$ defined by

$$g_k(z) = U_{z,z_0} g_k(z_0) = g_k(z_0) + (z - z_0)(A_1 - z)^{-1} g_k(z_0), \\ z \in \rho(A_1), \; k = 1, \dots, r,$$

forms a **basis** for $\ker(A_0^* - z)$.

$\{g_k(z)\}_{k=1}^r$ and $\{g_k(z')\}_{k=1}^r$ for $z, z' \in \rho(A_1)$ are **related** by

$$g_k(z') = U_{z',z} g_k(z) = g_k(z) + (z' - z)(A_1 - z')^{-1} g_k(z), \quad z, z' \in \rho(A_1).$$

Krein's Formula: Abstract Setting contd.

Theorem 2 (Krein's Formula)

For each $z \in \rho(A_1) \cap \rho(A_2)$, there is a unique, nonsingular, $r \times r$ **Nevanlinna–Herglotz** *matrix $P(z) = \big(p_{j,k}(z)\big)_{1 \leq j,k \leq r}$, depending on the choice of basis $\{g_k(z_0)\}_{k=1}^r$, such that*

$$\boxed{(A_2 - z)^{-1} = (A_1 - z)^{-1} + \sum_{j,k=1}^{r} p_{j,k}(z) (g_k(\overline{z}), \cdot)_{\mathcal{H}}\, g_j(z).}$$

$P(z)$ and $P(z')$ for $z, z' \in \rho(A_1) \cap \rho(A_2)$ are related by

$$P(z)^{-1} = P(z')^{-1} + (z - z')\big((g_j(\overline{z}), g_k(z'))_{\mathcal{H}}\big)_{1 \leq j,k \leq r}, \quad z, z' \in \rho(A_1) \cap \rho(A_2).$$

What about this **basis dependence** of the basic matrix $P(z)$?

Krein's Formula: Abstract Setting contd.

If $\{\widehat{g}_k(z_0)\}_{k=1}^r$ is any other basis for $\ker(A_0^* - z_0)$ and $\widehat{P}(z) = \big(\widehat{p}_{j,k}(z)\big)_{1\leq j,k\leq r}$ is the corresponding unique, nonsingular, $r \times r$ matrix-valued function such that

$$(A_2 - z)^{-1} = (A_1 - z)^{-1} + \sum_{j,k=1}^{r} \widehat{p}_{j,k}(z) (\widehat{g}_k(\overline{z}), \cdot)_{\mathcal{H}}\, \widehat{g}_j(z), \quad z \in \rho(A_1) \cap \rho(A_2),$$

then

$$\widehat{P}(z) = \big(T^{-1}\big)^{\top} P(z) \big((T^{-1})^{\top}\big)^{*},$$

where T is the $r \times r$ transition matrix corresponding to the change of basis from $\{g_k(z_0)\}_{k=1}^r$ to $\{\widehat{g}_k(z_0)\}_{k=1}^r$.

$S^{\top}$ denotes the transpose of S.

Krein's Formula: Schrödinger Operators on $(0, R)$

Reference self-adjoint extension: $H_{0,0}$, the **Dirichlet** extension of H_{min},

$$H_{0,0} f = \tau f, \quad f \in \operatorname{dom}(H_{0,0}) = \big\{ g \in \operatorname{dom}(H_{max}) \,\big|\, g(0) = 0 = g(R) \big\}.$$

For each $z \in \rho(H_{0,0})$, a basis for $\ker(H_{min}^* - z)$, denoted $\{u_j(z,\cdot)\}_{j=1,2}$, is fixed by specifying

$$\begin{array}{ll} u_1(z,0) = 0, \quad u_1(z,R) = 1, \\ u_2(z,0) = 1, \quad u_2(z,R) = 0, \end{array} \quad z \in \rho(H_{0,0}).$$

One verifies

$$\begin{array}{l} U_{z,z'} u_1(z',\cdot) = u_1(z,\cdot), \\ U_{z,z'} u_2(z',\cdot) = u_2(z,\cdot), \end{array} \quad j \in \{1,2\}, \ z, z' \in \rho(H_{0,0}),$$

where the generalized Cayley transform $U_{z,z'}$ of $H_{0,0}$ is defined by

$$\begin{aligned} U_{z,z'} &= (H_{0,0} - z')(H_{0,0} - z)^{-1} \\ &= I_{L^2((0,R);dx)} + (z - z')(H_{0,0} - z)^{-1}, \quad z, z' \in \rho(H_{0,0}), \end{aligned}$$

$$U_{z,z'} : \ker(H_{min}^* - z') \to \ker(H_{min}^* - z) \ \text{ is a bijection.}$$

Krein's Formula: Schrödinger Ops. on $(0, R)$ contd.

Case I: Separated boundary conditions, H_{θ_0,θ_R}:

Theorem 3

(i) If $\theta_0 \neq 0$ and $\theta_R \neq 0$, then the maximal common part of H_{θ_0,θ_R} and $H_{0,0}$ is $H_{\min}$. Assume $z \in \rho(H_{\theta_0,\theta_R}) \cap \rho(H_{0,0})$. Then the matrix

$$D_{\theta_0,\theta_R}(z) = \begin{pmatrix} \cot(\theta_R) - u_1'(z,R) & -u_2'(z,R) \\ u_1'(z,0) & \cot(\theta_0) + u_2'(z,0) \end{pmatrix},$$

is invertible and

$$\boxed{(H_{\theta_0,\theta_R} - z)^{-1} = (H_{0,0} - z)^{-1} - \sum_{j,k=1}^{2} D_{\theta_0,\theta_R}(z)^{-1}_{j,k} (u_k(\overline{z},\cdot),\cdot)_{L^2((0,R))}\, u_j(z,\cdot).}$$

Krein's Formula: Schrödinger Ops. on $(0,R)$ contd.

Theorem 3 (contd.)

(*ii*) If $\theta_0 \neq 0$, then the maximal common part of $H_{\theta_0,0}$ and $H_{0,0}$ is the restriction, $\widetilde{H}_{min}$, of H_{max} with domain

$$\operatorname{dom}\big(\widetilde{H}_{min}\big) = \operatorname{dom}(H_{max}) \cap \{g \in \mathrm{AC}([0,R]) \,|\, g(R) = g(0) = g'(0) = 0\}.$$

Assume $z \in \rho(H_{\theta_0,0}) \cap \rho(H_{0,0})$. Then $d_{\theta_0,0}(z) = \cot(\theta_0) + u_2'(z,0) \neq 0$ and

$$\boxed{(H_{\theta_0,0} - z)^{-1} = (H_{0,0} - z)^{-1} - d_{\theta_0,0}(z)^{-1} (u_2(\overline{z},\cdot),\cdot)_{L^2((0,R))}\, u_2(z,\cdot).}$$

(*iii*) If $\theta_R \neq 0$, then the maximal common part of H_{0,θ_R} and $H_{0,0}$ is the restriction, $\widehat{H}_{min}$, of H_{max} with domain

$$\operatorname{dom}\big(\widehat{H}_{min}\big) = \operatorname{dom}(H_{max}) \cap \{g \in \mathrm{AC}([0,R]) \,|\, g(R) = g(0) = g'(R) = 0\}.$$

Assume $z \in \rho(H_{0,\theta_R}) \cap \rho(H_{0,0})$. Then $d_{0,\theta_R}(z) = \cot(\theta_R) - u_1'(z,R) \neq 0$ and

$$\boxed{(H_{0,\theta_R} - z)^{-1} = (H_{0,0} - z)^{-1} - d_{0,\theta_R}(z)^{-1} (u_1(\overline{z},\cdot),\cdot)_{L^2((0,R))}\, u_1(z,\cdot).}$$

Krein's Formula: Schrödinger Ops. on $(0,R)$ contd.

Case II: Coupled boundary conditions, $H_{\phi,F}$:

Theorem 4

Let $F=(F_{j,k})_{1\leq j,k\leq 2}\in \mathrm{SL}(2,\mathbb{R})$, $\phi\in[0,2\pi)$, *and* $z\in\rho(H_{F,\phi})\cap\rho(H_{0,0})$.

(i) *If* $F_{1,2}\neq 0$, *then the maximal common part of* $H_{F,\phi}$ *and* $H_{0,0}$ *is* $H_{\min}$. *The matrix*

$$Q_{F,\phi}(z)=\begin{pmatrix} \frac{F_{2,2}}{F_{1,2}}-u_1'(z,R) & \frac{-1}{e^{-i\phi}F_{1,2}}-u_2'(z,R) \\ \frac{-1}{e^{i\phi}F_{1,2}}+u_1'(z,0) & \frac{F_{1,1}}{F_{1,2}}+u_2'(z,0) \end{pmatrix}$$

is invertible and

$$\boxed{(H_{F,\phi}-z)^{-1}=(H_{0,0}-z)^{-1}-\sum_{j,k=1}^{2}Q_{F,\phi}(z)^{-1}_{j,k}(u_k(\overline{z},\cdot),\cdot)_{L^2((0,R))}\,u_j(z,\cdot).}$$

Krein's Formula: Schrödinger Ops. on $(0, R)$ contd.

Theorem 4 (contd.)

Let $F = (F_{j,k})_{1\leq j,k\leq 2} \in \mathrm{SL}(2,\mathbb{R})$, $\phi \in [0, 2\pi)$, and $z \in \rho(H_{F,\phi}) \cap \rho(H_{0,0})$.

(ii) If $F_{1,2} = 0$, then the maximal common part of $H_{F,\phi}$ and $H_{0,0}$ is the restriction of $H_{\max}$ to the domain

$$\mathrm{dom}(H_{\max}) \cap \{g \in L^2((0,R);dx) \,|\, g(0) = g(R) = 0,\ g'(R) = e^{i\phi} F_{2,2} g'(0)\}.$$

In this case,

$$\begin{aligned} q_{F,\phi}(z) = F_{2,1}F_{2,2} + F_{2,2}^2 u_2'(z,0) + e^{i\phi} F_{2,2} u_1'(z,0) \\ - e^{-i\phi} F_{2,2} u_2'(z,R) - u_1'(z,R) \neq 0 \end{aligned}$$

and

$$\boxed{(H_{F,\phi} - z)^{-1} = (H_{0,0} - z)^{-1} - q_{F,\phi}(z)^{-1} (u_{F,\phi}(\overline{z},\cdot),\cdot)_{L^2((0,R))}\, u_{F,\phi}(z,\cdot).}$$

Here

$$u_{F,\phi}(z,\cdot) = e^{-i\phi} F_{2,2} u_2(z,\cdot) + u_1(z,\cdot).$$

Special Case: The Krein–von Neumann Extension

(I) Abstract Situation:

Let $\mathcal{H}$ be a separable complex Hilbert space with scalar product $(\cdot,\cdot)_{\mathcal{H}}$ and identity operator $I_{\mathcal{H}}$ in $\mathcal{H}$.

S denotes a **symmetric, closed, densely defined** operator in $\mathcal{H}$ **bounded from below** (typically, $S \geq 0$).

S_F denotes the **Friedrichs extension** of S.

S_K denotes the **Krein-von Neumann extension** of S.

$\dot{+}$ denotes the direct sum (not necessarily orthogonal) in $\mathcal{H}$.

A linear operator $T : \mathrm{dom}(T) \subseteq \mathcal{H} \to \mathcal{H}$ is called **non-negative**, $T \geq 0$, if

$$(u, Tu)_{\mathcal{H}} \geq 0, \quad u \in \mathrm{dom}(T).$$

T is called **strictly positive**, if for some $\varepsilon > 0$, $(u, Tu)_{\mathcal{H}} \geq \varepsilon \|u\|_{\mathcal{H}}^2$, $u \in \mathrm{dom}(T)$. One then writes $T \geq \varepsilon I_{\mathcal{H}}$. Similarly, one defines $T \geq S$ (but there are technical details concerning (quadratic form) domains........)

Mark G. Krein (1907–1989). His 1947 result

Theorem

$S \geq 0$ densely defined, closed in $\mathcal{H}$. Then, among all non-negative self-adjoint extensions of S, there exist two distinguished (really, extremal) ones, S_K and S_F, which are the smallest and largest (in the sense of order between the quadratic forms associated with self-adjoint operators) such extensions. Any non-negative self-adjoint extension $\widetilde{S} \geq 0$ of S necessarily satisfies

$$(S_F + t)^{-1} \leq (\widetilde{S} + t)^{-1} \leq (S_K + t)^{-1} \text{ for all } t > 0.$$

In particular, this determines S_K and S_F uniquely.
In addition, if $S \geq \varepsilon I_{\mathcal{H}}$ for some $\varepsilon > 0$, one has

$$\begin{aligned}
\operatorname{dom}(S_F) &= \operatorname{dom}(S) \dotplus (S_F)^{-1} \ker(S^*), \\
\operatorname{dom}(S_K) &= \operatorname{dom}(S) \dotplus \ker(S^*), \\
\operatorname{dom}(S^*) &= \operatorname{dom}(S) \dotplus (S_F)^{-1} \ker(S^*) \dotplus \ker(S^*), \\
\ker(S_K) &= \ker\big((S_K)^{1/2}\big) = \ker(S^*) = \operatorname{ran}(S)^{\perp} = \operatorname{def}(S),
\end{aligned}$$

this null space might be infinite-dimensional (e.g., for PDEs)!!!

Intrinsic Characterizations of S_F and S_K

Theorem (Freudenthal 1936; after Friedrichs '34)

Assume $S \geq 0$. Then,

$$S_F u := S^* u,$$
$$u \in \operatorname{dom}(S_F) := \big\{ v \in \operatorname{dom}(S^*) \,\big|\, \text{there exists } \{v_j\}_{j\in\mathbb{N}} \subset \operatorname{dom}(S),$$
$$\text{with } \lim_{j\to\infty} \|v_j - v\|_{\mathcal{H}} = 0 \text{ and } ((v_j - v_k), S(v_j - v_k))_{\mathcal{H}} \to 0 \text{ as } j,k \to \infty \big\}.$$

In addition, $S_F = S^*|_{\operatorname{dom}(S^*)\cap\operatorname{dom}((S_F)^{1/2})}$.

Theorem (Ando–Nishio 1970; after von Neumann '29–30 & M. Krein '47)

Assume $S \geq 0$. Then,

$$S_K u := S^* u,$$
$$u \in \operatorname{dom}(S_K) := \big\{ v \in \operatorname{dom}(S^*) \,\big|\, \text{there exists } \{v_j\}_{j\in\mathbb{N}} \subset \operatorname{dom}(S), \text{with}$$
$$\lim_{j\to\infty} \|S v_j - S^* v\|_{\mathcal{H}} = 0 \text{ and } ((v_j - v_k), S(v_j - v_k))_{\mathcal{H}} \to 0 \text{ as } j,k \to \infty \big\}.$$

The Krein–von Neumann Extension contd.

(II) Concrete Situation: Schrödinger Operators on $(0, R)$**:**

We recall that for each $z \in \rho(H_{0,0})$, $\{u_j(z,\cdot)\}_{j=1,2}$ is a basis for $\ker(H_{\min}^* - z)$, satisfying $u_1(z,0) = 0$, $u_1(z,R) = 1$, $u_2(z,0) = 1$, $u_2(z,R) = 0$, $z \in \rho(H_{0,0})$.

Theorem 5

Assume $z \in \rho(H_K) \cap \rho(H_{0,0})$. *Then* $H_K = H_{\phi_K, F_K}$ *and*

$$\boxed{(H_K - z)^{-1} = (H_{0,0} - z)^{-1} - \sum_{j,k=1}^{2} Q_{F_K,0}(z)_{j,k}^{-1} (u_k(\overline{z},\cdot),\cdot)_{L^2((0,R))}\, u_j(z,\cdot),}$$

where

$$\phi_K = 0, \quad F_K = \frac{1}{u_1'(0,0)} \begin{pmatrix} -u_2'(0,0) & 1 \\ u_1'(0,0)u_2'(0,R) - u_1'(0,R)u_2'(0,0) & u_1'(0,R) \end{pmatrix},$$

$$Q_{F_K,0}(z) = \begin{pmatrix} u_1'(0,R) - u_1'(z,R) & -u_1'(0,0) - u_2'(z,R) \\ -u_1'(0,0) + u_1'(z,0) & -u_2'(0,0) + u_2'(z,0) \end{pmatrix}.$$

The Krein–von Neumann Extension contd.

(III) Special Case: $V \equiv 0$ **on** $(0,R)$**, the Krein Laplacian** $H_{\mathbf{K}}^{(0)} = (-d^2/dx^2)_K$

In this case,

$$u_1^{(0)}(0,x) = \frac{x}{R}, \quad u_2^{(0)}(0,\cdot) = 1 - \frac{x}{R}, \quad x \in [0,R],$$

and the boundary conditions for the **Krein Laplacian** $H_{\mathrm{K}}^{(0)} = (-d^2/dx^2)_K$ then read

$$\begin{pmatrix} u(R) \\ u'(R) \end{pmatrix} = F_{\mathrm{K}}^{(0)} \begin{pmatrix} u(0) \\ u'(0) \end{pmatrix}, \quad u \in \operatorname{dom}\big(H_{\mathrm{K}}^{(0)}\big),$$

where

$$F_{\mathrm{K}}^{(0)} = \begin{pmatrix} 1 & R \\ 0 & 1 \end{pmatrix}.$$

Explicitly (cf., **Alonso and Simon 1980, Fukushima 1980**),

$$\boxed{u'(R) = u'(0) = [u(R) - u(0)]/R, \quad u \in \operatorname{dom}\big(H_{\mathrm{K}}^{(0)}\big).}$$

Who would have guessed that ....?

The Basics of Boundary Data Maps

Case (I): Robin-to-Robin Maps: Consider the **boundary trace map**

$$\gamma_{\theta_0,\theta_R}: \begin{cases} C^1([0,R]) \to \mathbb{C}^2, \\ u \mapsto \begin{pmatrix} \cos(\theta_0)u(0) + \sin(\theta_0)u'(0) \\ \cos(\theta_R)u(R) - \sin(\theta_R)u'(R) \end{pmatrix}. \end{cases} \qquad \theta_0, \theta_R \in [0,\pi),$$

For $z \in \mathbb{C}\backslash\sigma(H_{\theta_0,\theta_R})$ and $\theta_0, \theta_R \in [0,\pi)$, the boundary value problem

$$-u'' + Vu = zu, \quad u, u' \in AC([0,R]), \quad \gamma_{\theta_0,\theta_R}(u) = \begin{pmatrix} c_0 \\ c_R \end{pmatrix} \in \mathbb{C}^2,$$

has a unique solution $u(z,\cdot) = u(z,\cdot\,; (\theta_0,c_0),(\theta_R,c_R))$ for each $c_0, c_R \in \mathbb{C}$.

To each such boundary value problem, we now associate a family of **general boundary data**, or **Robin-to-Robin maps**,

$$\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z) : \mathbb{C}^2 \to \mathbb{C}^2, \quad \theta_0, \theta_R, \theta_0', \theta_R' \in [0,\pi), \; z \in \mathbb{C}\backslash\sigma(H_{\theta_0,\theta_R}),$$

$$\begin{aligned} \Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\begin{pmatrix} c_0 \\ c_R \end{pmatrix} &= \Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\big(\gamma_{\theta_0,\theta_R}(u(z,\cdot\,;(\theta_0,c_0),(\theta_R,c_R)))\big) \\ &= \gamma_{\theta_0',\theta_R'}(u(z,\cdot\,;(\theta_0,c_0),(\theta_R,c_R))). \end{aligned}$$

The Basics of Boundary Data Maps contd.

With $u(z,\cdot) = u(z,\cdot\,;(\theta_0, c_0),(\theta_R, c_R))$, $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)$ can be represented as the 2×2 complex matrix,

$$\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\begin{pmatrix} c_0 \\ c_R \end{pmatrix} = \Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\begin{pmatrix} \cos(\theta_0)u(z,0) + \sin(\theta_0)u'(z,0) \\ \cos(\theta_R)u(z,R) - \sin(\theta_R)u'(z,R) \end{pmatrix}$$
$$= \begin{pmatrix} \cos(\theta_0')u(z,0) + \sin(\theta_0')u'(z,0) \\ \cos(\theta_R')u(z,R) - \sin(\theta_R')u'(z,R) \end{pmatrix}.$$

The Basics of Boundary Data Maps contd.

The Dirichlet trace γ_D, and the Neumann trace γ_N (in connection with the outward pointing unit normal vector at $\partial(0,R) = \{0,R\}$), are given by

$$\gamma_D = \gamma_{0,0} = -\gamma_{\pi,\pi}, \quad \gamma_N = \gamma_{3\pi/2,3\pi/2} = -\gamma_{\pi/2,\pi/2}.$$

The **Dirichlet-to-Neumann map,** $\Lambda_{D,N}(z)$, corresponds to $\theta_0 = \theta_R = 0$, $\theta_0' = \theta_R' = \pi/2$,

$$\boxed{\Lambda_{D,N}(z)\begin{pmatrix} u(z,0) \\ u(z,R) \end{pmatrix} = \Lambda_{0,0}^{\frac{\pi}{2},\frac{\pi}{2}}(z)\begin{pmatrix} u(z,0) \\ u(z,R) \end{pmatrix} = \begin{pmatrix} u'(z,0) \\ -u'(z,R) \end{pmatrix}, \quad z \in \mathbb{C}\backslash\sigma(H_{0,0}).}$$

Note. If $V = 0$, the **Dirichlet-to-Neumann map** has been considered in Example 5.1 of **Posilicano, OaM 2, 483–506 (2008).**
The **Neumann-to-Dirichlet map**

$$\Lambda_{N,D}(z) = \Lambda_{\pi/2,\pi/2}^{\pi,\pi}(z) = -[\Lambda_{D,N}(z)]^{-1}$$

in the case $V = 0$ has been computed earlier in Example 4.1 of **V. Derkach and M. Malamud,** Ukrain. Math. J. **44**, 379–401 (1992).

The Basics of Boundary Data Maps contd.

Next we unify separated and coupled boundary conditions:

Theorem 6 (e.g., Weidmann 2003 (German edition), Thm. 13.14)

The operator $H_{A,B}$,

$$H_{A,B} f = \tau f, \quad f \in \mathrm{dom}(H_{A,B}) = \left\{ g \in \mathrm{dom}(H_{\max}) \,\middle|\, A \begin{pmatrix} g(0) \\ g'(0) \end{pmatrix} = B \begin{pmatrix} g(R) \\ g'(R) \end{pmatrix} \right\},$$

is a self-adjoint extension of $H_{\min}$ *if and only if there exist matrices* $A, B \in \mathbb{C}^{2\times 2}$ *satisfying* $\mathrm{rank}(A \;\; B) = 2$, $AJA^* = BJB^*$, $J = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$.

In particular, the case of separated boundary conditions corresponds to

$$A = \begin{pmatrix} \cos(\theta_0) & \sin(\theta_0) \\ 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 \\ -\cos(\theta_R) & \sin(\theta_R) \end{pmatrix}, \quad \theta_0, \theta_R \in [0, \pi).$$

The case of coupled (i.e., non-separated) boundary conditions corresponds to

$$A = e^{i\phi} F, \quad B = I_2, \quad F \in \mathrm{SL}(2, \mathbb{R}), \; \phi \in [0, 2\pi).$$

The Basics of Boundary Data Maps contd.

Case (II): General Boundary Data Maps:

Define the **general boundary trace map,** $\gamma_{A,B}$, associated with the boundary $\{0,R\}$ of $(0,R)$ and the 2×2 parameter matrices A, B satisfying $\operatorname{rank}(A \;\; B) = 2$, $AJA^* = BJB^*$, $J = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$, by

$$\gamma_{A,B} : \begin{cases} C^1([0,R]) \to \mathbb{C}^2, \\ u \mapsto A \begin{pmatrix} u(0) \\ u'(0) \end{pmatrix} - B \begin{pmatrix} u(R) \\ u'(R) \end{pmatrix}. \end{cases}$$

Then,

$$\gamma_{A,B} = D_{A,B}\gamma_D + N_{A,B}\gamma_N, \quad D_{A,B} = \begin{pmatrix} A_{1,1} & -B_{1,1} \\ A_{2,1} & -B_{2,1} \end{pmatrix}, \; N_{A,B} = \begin{pmatrix} A_{1,2} & B_{1,2} \\ A_{2,2} & B_{2,2} \end{pmatrix}.$$

Moreover, define

$$S_{A',B',A,B} = N_{A',B'}D_{A,B}^* - D_{A',B'}N_{A,B}^*.$$

The Basics of Boundary Data Maps contd.

Let $A, B \in \mathbb{C}^{2\times 2}$ be such that $\operatorname{rank}(A \;\; B) = 2$, and assume that $z \in \rho(H_{A,B})$. Then the boundary value problem

$$-u'' + Vu = zu, \quad u, u' \in AC([0, R]), \quad \gamma_{A,B} u = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \in \mathbb{C}^2,$$

has a unique solution $u(z, \cdot) = u_{A,B}(z, \cdot\,; c_1, c_2)$ for each $c_1, c_2 \in \mathbb{C}$.

Let $A, B, A', B' \in \mathbb{C}^{2\times 2}$ with A, B satisfying $\operatorname{rank}(A \;\; B) = 2$, $AJA^* = BJB^*$, $J = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$, and similarly for A', B'. Assuming $z \in \rho(H_{A,B})$, we introduce the **general boundary data map** by

$$\begin{aligned} &\Lambda_{A,B}^{A',B'}(z) : \mathbb{C}^2 \to \mathbb{C}^2, \\ &\Lambda_{A,B}^{A',B'}(z) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \Lambda_{A,B}^{A',B'}(z)\, \gamma_{A,B} u_{A,B}(z, \cdot\,; c_1, c_2) \\ &\qquad\qquad\qquad\qquad = \gamma_{A',B'} u_{A,B}(z, \cdot\,; c_1, c_2), \end{aligned}$$

where $u_{A,B}(z, \cdot; c_1, c_2)$ satisfies the above boundary value problem.

The Basics of Boundary Data Maps contd.

Basis Properties of $\Lambda_{A,B}^{A',B'}(z)$:

$$\Lambda_{A,B}^{A',B'}(z) = D_{A',B'}\Lambda_{A,B}^{D}(z) + N_{A',B'}\Lambda_{A,B}^{N}(z), \quad z \in \rho(H_{A,B}),$$
$$\Lambda_{A,B}^{A,B}(z) = I_2, \quad z \in \rho(H_{A,B}),$$
$$\Lambda_{A',B'}^{A'',B''}(z)\,\Lambda_{A,B}^{A',B'}(z) = \Lambda_{A,B}^{A'',B''}(z), \quad z \in \rho(H_{A,B}) \cap \rho(H_{A',B'}),$$
$$\Lambda_{A,B}^{A',B'}(z) = \left[\Lambda_{A',B'}^{A,B}(z)\right]^{-1}, \quad z \in \rho(H_{A,B}) \cap \rho(H_{A',B'}).$$

Resolvent Connection:

Theorem 7

Let $A, B, A', B' \in \mathbb{C}^{2\times 2}$ with A, B satisfying $\operatorname{rank}(A \;\; B) = 2$, $AJA^* = BJB^*$, $J = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$, and similarly for A', B'.

$$\boxed{\Lambda_{A,B}^{A',B'}(z)S_{A',B',A,B}^{*} = \gamma_{A',B'}\left[\gamma_{A',B'}(H_{A,B} - \bar{z})^{-1}\right]^{*}, \quad z \in \rho(H_{A,B}).}$$

In particular, $\Lambda_{A,B}^{A',B'}(\cdot)S_{A',B',A,B}^{*}$ is a Nevanlinna–Herglotz matrix (i.e., analytic on $\mathbb{C}_+$ with nonnegative imaginary part on $\mathbb{C}_+$).

Krein's Formula and Boundary Data Maps

Corollary 8

Let $A, B \in \mathbb{C}^{2\times 2}$ *and* $A', B' \in \mathbb{C}^{2\times 2}$ *satisfy* $\operatorname{rank}(A \quad B) = 2$, $AJA^* = BJB^*$, $J = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$, *and similarly for* A', B', *and let* $z \in \rho(H_{A,B}) \cap \rho(H_{A',B'})$.

(i) *If* $S_{A',B',A,B}$ *is invertible* $($*i.e.*, $\operatorname{rank}(S_{A',B',A,B}) = 2)$, *then*

$$\boxed{\begin{aligned}(H_{A',B'} - z)^{-1} &= (H_{A,B} - z)^{-1} \\ &\quad - \sum_{k,n=1}^{2} P(z)^{-1}_{k,n} (g_n(\overline{z}, \cdot), \cdot)_{L^2((0,R))}\, g_k(z, \cdot),\end{aligned}}$$

where the 2×2 *matrix* $P(z)$ *is given by*

$$P(z) = {S_{A',B',A,B}}^{-1} \Lambda_{A,B}^{A',B'}(z)$$

and $\{g_1(z, \cdot), g_2(z, \cdot)\}$ *is the basis of* $\ker(H_{\max} - z)$ *satisfying the boundary conditions* $\gamma_{A,B}\, g_1(z, \cdot) = (1, 0)^\top$ *and* $\gamma_{A,B}\, g_2(z, \cdot) = (0, 1)^\top$.

Krein's Formula and Boundary Data Maps contd.

Corollary 8 (contd.)

Let $A, B \in \mathbb{C}^{2\times 2}$ and $A', B' \in \mathbb{C}^{2\times 2}$ satisfy $\operatorname{rank}(A \;\; B) = 2$, $AJA^* = BJB^*$, $J = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$, and similarly for A', B', and let $z \in \rho(H_{A,B}) \cap \rho(H_{A',B'})$.

(ii) If $S_{A',B',A,B}$ is not invertible and nonzero (i.e., $\operatorname{rank}(S_{A',B',A,B}) = 1$), then

$$\boxed{(H_{A',B'} - z)^{-1} = (H_{A,B} - z)^{-1} - p(z)^{-1}(g_0(\overline{z}), \cdot)_{L^2((0,R))}\, g_0(z),}$$

where the scalar $p(z)$ is given by

$$p(z) = P_{\operatorname{ran}(S_{A',B',A,B})} \Lambda_{A,B}^{A',B'}(z) S_{A',B',A,B}^* P_{\operatorname{ran}(S_{A',B',A,B})}\big|_{\operatorname{ran}(S_{A',B',A,B})}$$

and the function $g_0(z, \cdot) \in \ker(H_{\max} - z)$ is given by

$$g_0(z, \cdot) = \left[\gamma_{A',B'}(H_{A,B} - \overline{z})^{-1}\right]^*\big|_{\operatorname{ran}(S_{A',B',A,B})}.$$

BD Maps and Krein's Resolvent Formula Revisited

Theorem 9

Let $A, B \in \mathbb{C}^{2\times 2}$ *and* $A', B' \in \mathbb{C}^{2\times 2}$ *satisfy* $\operatorname{rank}(A \;\; B) = 2$, $AJA^* = BJB^*$, $J = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$, *and similarly for* A', B', *and let* $z \in \rho(H_{A,B}) \cap \rho(H_{A',B'})$.

(*i*) *If* $S_{A',B',A,B}$ *is invertible* (*i.e.*, $\operatorname{rank}(S_{A',B',A,B}) = 2$), *then*

$$\boxed{\begin{aligned}(H_{A',B'} - z)^{-1} &= (H_{A,B} - z)^{-1} \\ &\quad - \big[\gamma_{A',B'}(H_{A,B} - \bar{z})^{-1}\big]^* \big[\Lambda_{A,B}^{A',B'}(z) S^*_{A',B',A,B}\big]^{-1} \big[\gamma_{A',B'}(H_{A,B} - z)^{-1}\big].\end{aligned}}$$

(*ii*) *If* $S_{A',B',A,B}$ *is not invertible and nonzero* (*i.e.*, $\operatorname{rank}(S_{A',B',A,B}) = 1$), *then*

$$\boxed{\begin{aligned}(H_{A',B'} - z)^{-1} &= (H_{A,B} - z)^{-1} \\ &\quad - \big[\gamma_{A',B'}(H_{A,B} - \bar{z})^{-1}\big]^* \big[\lambda_{A,B}^{A',B'}(z)\big]^{-1} \big[\gamma_{A',B'}(H_{A,B} - z)^{-1}\big],\end{aligned}}$$

where

$$\lambda_{A,B}^{A',B'}(z) = P_{\operatorname{ran}(S_{A',B',A,B})} \Lambda_{A,B}^{A',B'}(z) S^*_{A',B',A,B} P_{\operatorname{ran}(S_{A',B',A,B})}\big|_{\operatorname{ran}(S_{A',B',A,B})}.$$

BD Maps, Fredholm Dets., and Trace Formulas

The connection between **BD maps, trace formulas, and symmetrized perturbation determinants:**

Let $e_0 = \inf\big(\sigma(H_{A,B}) \cup \sigma(H_{A',B'})\big)$.

Theorem 10

Let $A, B \in \mathbb{C}^{2\times 2}$ *and* $A', B' \in \mathbb{C}^{2\times 2}$ *satisfy* $\operatorname{rank}(A \;\; B) = 2$, $AJA^* = BJB^*$, $J = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$, *and similarly for* A', B'. *Then, for* $z \in \mathbb{C}\backslash[e_0, \infty)$,

$$\boxed{\operatorname{tr}_{L^2((0,R);dx)}\left(\left(H_{A',B'} - z\right)^{-1} - \left(H_{A,B} - z\right)^{-1}\right) = -\frac{d}{dz}\ln\left(\det_{\mathbb{C}^2}\left(\Lambda_{A,B}^{A',B'}(z)\right)\right).}$$

Perhaps, the most compelling reason to study $\boldsymbol{\Lambda_{A,B}^{A',B'}(z)}$ ....

BD Maps, Fredholm Dets., and Trace Formulas

Let $e_0 = \inf\big(\sigma(H_{A,B}) \cup \sigma(H_{A',B'})\big)$.

Theorem 10 (contd.)

Let $A, B \in \mathbb{C}^{2\times 2}$ and $A', B' \in \mathbb{C}^{2\times 2}$ satisfy $\operatorname{rank}(A \;\; B) = 2$, $AJA^* = BJB^*$, $J = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$, and similarly for A', B'. Then, for $z \in \mathbb{C}\backslash[e_0, \infty)$,

$$\begin{aligned}
&\det{}_{L^2((0,R);dx)}\Big(\overline{(H_{A',B'} - z)^{1/2}(H_{A,B} - z)^{-1}(H_{A',B'} - z)^{1/2}}\Big) \\
&\quad = \frac{\det_{\mathbb{C}^2}(N_{A,B})}{\det_{\mathbb{C}^2}(N_{A',B'})} \det{}_{\mathbb{C}^2}\Big(\Lambda_{A,B}^{A',B'}(z)\Big), \quad \det{}_{\mathbb{C}^2}(N_{A',B'}) \neq 0, \\
&\operatorname{tr}_{L^2((0,R);dx)}\big((H_{A',B'} - z)^{-1} - (H_{A,B} - z)^{-1}\big) \\
&\quad = -\frac{d}{dz} \ln\Big(\det{}_{L^2((0,R);dx)}\Big(\overline{(H_{A',B'} - z)^{1/2}(H_{A,B} - z)^{-1}(H_{A',B'} - z)^{1/2}}\Big)\Big) \\
&\quad = -\frac{d}{dz} \ln\Big(\det{}_{\mathbb{C}^2}\Big(\Lambda_{A,B}^{A',B'}(z)\Big)\Big), \quad \det{}_{\mathbb{C}^2}(N_{A,B}) \det{}_{\mathbb{C}^2}(N_{A',B'}) \neq 0.
\end{aligned}$$

BD Maps and Spectral Shift Functions

Since $\left[(H_{A',B'} - z)^{-1} - (H_{A,B} - z)^{-1}\right]$ is at most of **rank-two**, the **spectral shift function,** $\xi(\cdot; H_{A',B'}, H_{A,B})$, associated with the pair $(H_{A',B'}, H_{A,B})$ is well-defined.

Using the standard normalization,

$$\xi(\,\cdot\,; H_{A',B'}, H_{A,B}) = 0, \quad \lambda < e_0 = \inf\big(\sigma(H_{A,B}) \cup \sigma(H_{A',B'})\big),$$

Krein's trace formula reads

$$\begin{aligned}&\operatorname{tr}_{L^2((0,R);dx)}\big((H_{A',B'} - z)^{-1} - (H_{A,B} - z)^{-1}\big)\\ &\quad = -\int_{[e_0,\infty)} \frac{\xi(\lambda; H_{A',B'}, H_{A,B})\, d\lambda}{(\lambda - z)^2}, \quad z \in \rho(H_{A,B}) \cap \rho(H_{A',B'}),\end{aligned}$$

where

$$\xi(\cdot\,; H_{A',B'}, H_{A,B}) \in L^1\big(\mathbb{R}; (\lambda^2 + 1)^{-1} d\lambda\big). \tag{5.1}$$

BD Maps and Spectral Shift Functions contd.

Since the spectra of $H_{A,B}$ and $H_{A',B'}$ are **purely discrete**, $\xi(\,\cdot\,; H_{A',B'}, H_{A,B})$ is an **integer-valued piecewise constant** function on $\mathbb{R}$ with jumps precisely at the eigenvalues of $H_{A,B}$ and $H_{A',B'}$. In particular, $\xi(\,\cdot\,; H_{A',B'}, H_{A,B})$ represents the difference of the **eigenvalue counting** functions of $H_{A',B'}$ and $H_{A,B}$.

Theorem 11

Let $A, B \in \mathbb{C}^{2\times 2}$ and $A', B' \in \mathbb{C}^{2\times 2}$ satisfy $\mathrm{rank}(A \quad B) = 2$, $AJA^* = BJB^*$, $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, *and similarly for A', B'. Then, for a.e. $\lambda \in \mathbb{R}$,*

$$\xi(\lambda; H_{A',B'}, H_{A,B}) = \pi^{-1} \lim_{\varepsilon \downarrow 0} \mathrm{Im}\left(\ln\left(\eta_{A',B',A,B}\, \mathrm{det}_{\mathbb{C}^2}\left(\Lambda_{A,B}^{A',B'}(\lambda + i\varepsilon)\right)\right)\right),$$

where $\eta_{A',B',A,B} = e^{i\theta_{A',B',A,B}}$ for some $\theta_{A',B',A,B} \in [0, 2\pi)$.

BD Maps and Inverse Spectral Problems

A special case of separated boundary conditions: Define

$$\Lambda_{\theta_0,\theta_R}(z) = \Lambda_{\theta_0,\theta_R}^{(\theta_0+\frac{\pi}{2}) \bmod (2\pi), (\theta_R+\frac{\pi}{2}) \bmod (2\pi)}(z), \quad \theta_0, \theta_R \in [0,\pi), \quad z \in \mathbb{C}\backslash\sigma(H_{\theta_0,\theta_R}),$$

a generalization of the **Dirichlet-to-Neumann map**

$$\Lambda_{D,N}(z) = \Lambda_{0,0}^{\frac{\pi}{2},\frac{\pi}{2}}(z) \equiv \Lambda_{0,0}(z), \quad z \in \mathbb{C}\backslash\sigma(H_{0,0}).$$

Introduce the **Weyl–Titchmarsh *m*-functions** with the reference point the left/right endpoint 0, resp., R, denoted by $m_{+,\theta_0}(z,\theta_R)$, resp., $m_{-,\theta_R}(z,\theta_0)$.

Then $m_{+,\theta_0}(\cdot,\theta_R)$ and $-m_{-,\theta_R}(\cdot,\theta_0)$ are **Nevanlinna–Herglotz** functions and **asymptotically**,

$$\begin{aligned}
m_{+,\theta_0}(z,\theta_R) &\underset{z\to i\infty}{\longrightarrow} \cot(\theta_0) + o(1), \quad \theta_0 \in (0,\pi),\\
m_{+,0}(z,\theta_R) &\underset{z\to i\infty}{\longrightarrow} iz^{1/2} + o\big(z^{1/2}\big),\\
m_{-,\theta_R}(z,\theta_0) &\underset{z\to i\infty}{\longrightarrow} -\cot(\theta_R) + o(1), \quad \theta_R \in (0,\pi),\\
m_{-,0}(z,\theta_0) &\underset{z\to i\infty}{\longrightarrow} -iz^{1/2} + o\big(z^{1/2}\big).
\end{aligned}$$

BD Maps and Inverse Spectral Problems contd.

Theorem 12

Assume that $\theta_0, \theta_R \in [0, \pi)$. Then each diagonal entry of $\Lambda_{\theta_0,\theta_R}(z)$ (i.e., $\Lambda_{\theta_0,\theta_R}(z)_{1,1}$ or $\Lambda_{\theta_0,\theta_R}(z)_{2,2}$) uniquely determines H_{θ_0,θ_R}, that is, it uniquely determines $V(\cdot)$ a.e. on $(0, R)$, and also θ_0 and θ_R.

Proof.

It suffices to note the identity

$$\Lambda_{\theta_0,\theta_R}(z) = \begin{pmatrix} m_{+,\theta_0}(z, \theta_R) & \Lambda_{\theta_0,\theta_R}(z)_{1,2} \\ \Lambda_{\theta_0,\theta_R}(z)_{2,1} & -m_{-,\theta_R}(z, \theta_0) \end{pmatrix}$$

(where $\Lambda_{\theta_0,\theta_R}(z)_{1,2} = \Lambda_{\theta_0,\theta_R}(z)_{2,1}$ .....), and apply **Marchenko's fundamental 1952 uniqueness result** **(transl. 1973)** formulated in terms of m-functions. $\square$

Note. This is in **stark contrast** to the usual 2×2 matrix **Weyl–Titchmarsh M**-matrix!

BD Maps and Inverse Spectral Problems contd.

This has instant consequences for **Borg**-type (**Levinson**, etc.) **uniqueness results** (such as, **two spectra uniquely determine $\mathbf{H}_{\theta_0,\theta_R}$**, etc.).

Conjecture 13

The role $m_{+,\theta_0}(\cdot,\theta_R)$ (resp., $m_{-,\theta_R}(\cdot,\theta_0)$) plays for uniqueness results in the case of separated boundary conditions in connection with H_{θ_0,θ_R}, in general, is played by the boundary data map $\Lambda_{A,B}^{A'(A,B),B'(A,B)}(\cdot)$ (for a very particular choice of A', B' as a function of A, B) in the case of general boundary conditions in connection with $H_{A,B}$.

Note. For general boundary conditions indexed by A, B, one now can have multiplicity-two eigenvalues (as in the (anti)periodic cases), in sharp contrast to separated boundary conditions. Hence, more than one diagonal entry of $\Lambda_{A,B}^{A'(A,B),B'(A,B)}(\cdot)$ will be involved in general.

SSF and D-N Maps: Motivation

• Hint at an extension of SSF, the Spectral Shift Operator (SSO), whose trace equals SSF.

• Connect SSO with abstract Weyl–Titchmarsh M-operators.

• Sketch applications to Dirichlet-to-Neumann maps for PDEs.

Based to a large extent on:

J. Behrndt, F.G., and S. Nakamura, *Spectral shift functions and Dirichlet-to-Neumann maps*, arXiv:1609.08292.

A quick SSF Summary:

General Hypothesis.

$\mathcal{H}$ a complex, separable Hilbert space, A, B self-adjoint (generally, unbounded) operators in $\mathcal{H}$.

I. M. Lifshitz, 1952.

$B - A$ **finite rank** operator. Then exists $\xi(\,\cdot\,; B, A) : \mathbb{R} \to \mathbb{R}$ such that *formally*,

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

Mark Krein and SSF, 1953–1962:

Theorem.

Assume $(B-A)$ is a **trace class** operator, i.e., $(B-A) \in \mathcal{B}_1(\mathcal{H})$. Then exists a real-valued $\xi(\,\cdot\,; B, A) \in L^1(\mathbb{R})$ such that

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

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

- $\operatorname{tr}_{\mathcal{H}}\big(\varphi(B) - \varphi(A)\big) = \int_{\mathbb{R}} \varphi'(\lambda)\xi(\lambda; B, A)\, d\lambda$ for $\varphi(\lambda) = (\lambda - z)^{-1}$.
- Extends to Wiener class $W_1(\mathbb{R})$: $\varphi'(\lambda) = \int e^{-i\lambda\mu}\, d\sigma(\mu)$.

Corollary.

If $\delta = (a, b)$ and $\overline{\delta} \cap \sigma_{\rm ess}(A) = \emptyset$ then

$$\xi(b-; B, A) - \xi(a+; B, A) = \dim(\mathrm{ran}(E_B(\delta))) - \dim(\mathrm{ran}(E_A(\delta))).$$

- Spectral shift function for U, V unitary, $(V - U) \in \mathcal{B}_1(\mathcal{H})$.

Mark Krein and SSF, 1953–1962 (contd.):

Theorem.

Assume

$$\big[(B - zI_{\mathcal{H}})^{-1} - (A - zI_{\mathcal{H}})^{-1}\big] \in \mathcal{B}_1(\mathcal{H}), \quad z \in \rho(A) \cap \rho(B). \qquad (*)$$

Then exists $\xi(\,\cdot\,; B, A) \in L^1_{\text{loc}}(\mathbb{R})$ such that $\int_{\mathbb{R}} |\xi(\lambda; B, A)|(1 + \lambda^2)^{-1}\, d\lambda < \infty$ and

$$\operatorname{tr}_{\mathcal{H}}\big((B - zI_{\mathcal{H}})^{-1} - (A - zI_{\mathcal{H}})^{-1}\big) = -\int_{\mathbb{R}} \frac{\xi(\lambda; B, A)\, d\lambda}{(\lambda - z)^2}, \quad z \in \rho(A) \cap \rho(B).$$

The function $\xi(\,\cdot\,; B, A)$ is unique up to a real constant.

- Trace formula for $\varphi(\lambda) = (\lambda - z)^{-1}$ and $\varphi(\lambda) = (\lambda - z)^{-k}$.
- Large class of φ's in trace formula in **Peller '85**.

Birman–Krein formula.

Assume $(*)$. The scattering matrix $\{S(\lambda; B, A)\}_{\lambda \in \sigma_{ac}(A)}$ for the pair (B, A) satisfies

$$\det(S(\lambda; B, A)) = e^{-2\pi i \xi(\lambda; B, A)} \quad \text{for a.e. } \lambda \in \sigma_{ac}(A).$$

SSF: Generalizations

L. S. Koplienko '71.

Assume $\rho(A) \cap \rho(B) \cap \mathbb{R} \neq \emptyset$ and for some $m \in \mathbb{N}$,

$$\big[(B - zI_{\mathcal{H}})^{-m} - (A - zI_{\mathcal{H}})^{-m}\big] \in \mathcal{B}_1(\mathcal{H}). \qquad (**)$$

Then exists $\xi(\,\cdot\,; B, A) \in L^1_{\mathrm{loc}}(\mathbb{R})$ such that $\int_{\mathbb{R}} |\xi(\lambda; B, A)|(1 + |\lambda|)^{-(m+1)}\, d\lambda < \infty$ and

$$\operatorname{tr}_{\mathcal{H}}\big((B - zI_{\mathcal{H}})^{-m} - (A - zI_{\mathcal{H}})^{-m}\big) = \int_{\mathbb{R}} \frac{-m}{(\lambda - z)^{m+1}}\, \xi(\lambda; B, A)\, d\lambda, \quad z \in \rho(A) \cap \rho(B).$$

D. R. Yafaev '05.

Assume $(**)$ for some $m \in \mathbb{N}$ odd. Then exists $\xi(\,\cdot\,; B, A) \in L^1_{\mathrm{loc}}(\mathbb{R})$ such that $\int_{\mathbb{R}} |\xi(\lambda; B, A)|(1 + |\lambda|)^{-(m+1)}\, d\lambda < \infty$

$$\operatorname{tr}_{\mathcal{H}}\big((B - zI_{\mathcal{H}})^{-m} - (A - zI_{\mathcal{H}})^{-m}\big) = \int_{\mathbb{R}} \frac{-m}{(\lambda - z)^{m+1}}\, \xi(\lambda; B, A)\, d\lambda, \quad z \in \rho(A) \cap \rho(B).$$

Note. Yafaev assumes **no** spectral gaps of A ($\longrightarrow$ **massless** Dirac-type operators).

Quasi Boundary Triples:

$S \subset S^*$ closed symmetric operator in $\mathcal{H}$, $n_+(S) = n_-(S) = \infty$.

Def. (Bruk '76, Kochubei '75; Derkach–Malamud '95; Behrndt–Langer '07)

$\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ **quasi boundary triple for S^*** if $\mathcal{G}$ Hilbert space and $T \subset \overline{T} = S^*$ and $\Gamma_0, \Gamma_1 : \mathrm{dom}(T) \to \mathcal{G}$ such that

(i) $(Tf, g) - (f, Tg) = (\Gamma_1 f, \Gamma_0 g) - (\Gamma_0 f, \Gamma_1 g)$, $f, g \in \mathrm{dom}(T)$.

(ii) $\Gamma := \begin{pmatrix} \Gamma_0 \\ \Gamma_1 \end{pmatrix} : \mathrm{dom}(T) \to \mathcal{G} \times \mathcal{G}$ dense range.

(iii) $A_0 = T \upharpoonright \ker(\Gamma_0)$ self-adjoint.

Example. ($-\Delta + V$ on domain Ω, $\partial\Omega$ of class C^2, $V \in L^\infty(\Omega)$ real-valued)

$$Sf = -\Delta f + Vf \upharpoonright \big\{f \in H^2(\Omega) \,\big|\, f|_{\partial\Omega} = \partial_\nu f|_{\partial\Omega} = 0\big\},$$

$$S^* f = -\Delta f + Vf \upharpoonright \big\{f \in L^2(\Omega) \,\big|\, \Delta f \in L^2(\Omega)\big\},$$

$$Tf = -\Delta f + Vf \upharpoonright H^2(\Omega).$$

Here $(Tf, g) - (f, Tg) = (f|_{\partial\Omega}, \partial_\nu g|_{\partial\Omega}) - (\partial_\nu f|_{\partial\Omega}, g|_{\partial\Omega})$.

Choose $\mathcal{G} = L^2(\partial\Omega)$, $\Gamma_0 f := \partial_\nu f|_{\partial\Omega}$, $\Gamma_1 f := f|_{\partial\Omega}$.

γ-Field and Weyl–Titchmarsh Function:

$S \subset T \subset \overline{T} = S^*$, $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ a quasi boundary triple (QBT).

Definition.

Let $f_z \in \ker(T - zI_{\mathcal{H}})$, $z \in \mathbb{C}\backslash\mathbb{R}$. **$\gamma$-field** and **Weyl–Titchmarsh M-function**:

$$\gamma(z) : \mathcal{G} \to \mathcal{H}, \quad \Gamma_0 f_z \mapsto f_z, \quad z \in \mathbb{C}\backslash\mathbb{R},$$

$$M(z) : \mathcal{G} \to \mathcal{G}, \quad \Gamma_0 f_z \mapsto \Gamma_1 f_z, \quad z \in \mathbb{C}\backslash\mathbb{R}.$$

- $\gamma(z)$ solves boundary value problem in PDE.
- $M(z)$ Dirichlet-to-Neumann in PDE.

Example. $(-\Delta + V$, QBT $\{L^2(\partial\Omega), \partial_\nu f|_{\partial\Omega}, f|_{\partial\Omega}\})$

Here $\ker(T - zI_{\mathcal{H}}) = \big\{f \in H^2(\Omega) \,\big|\, -\Delta f + Vf = zf\big\}$ and

$$\gamma(z) : L^2(\partial\Omega) \supset H^{1/2}(\partial\Omega) \to L^2(\Omega), \quad \varphi \mapsto f_z,$$

where $(-\Delta + V)f_z = zf_z$ and $\partial_\nu f_z|_{\partial\Omega} = \varphi$, and

$$M(z) : L^2(\partial\Omega) \supset H^{1/2}(\partial\Omega) \to L^2(\partial\Omega), \quad \varphi = \partial_\nu f_z|_{\partial\Omega} \mapsto f_z|_{\partial\Omega}.$$

Quasi Boundary Triples and Self-Adjoint Extensions:

Perturbation problems for self-adjoint operators in the QBT scheme:

Lemma.

Assume A, B self-adjoint in $\mathcal{H}$ and $S = A \cap B$, i.e.,

$$Sf := Af = Bf, \quad \operatorname{dom}(S) = \big\{ f \in \operatorname{dom}(A) \cap \operatorname{dom}(B) \,\big|\, Af = Bf \big\}$$

densely defined. Then there exists $T \subset \overline{T} = S^*$ and QBT $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ such that

$$A = T \restriction \ker(\Gamma_0) \ \text{ and } \ B = T \restriction \ker(\Gamma_1),$$

and

$$(B - zI_{\mathcal{H}})^{-1} - (A - zI_{\mathcal{H}})^{-1} = -\,\gamma(z) M(z)^{-1} \gamma(\bar{z})^*,$$

where γ and M are the **γ-field** and **Weyl–Titchmarsh function** of $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$.

Main Abstract Result: First-Order Case

Theorem.

A, B self-adjoint, $S = A \cap B$ densely defined, and $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ a QBT, $A = T \restriction \ker(\Gamma_0)$, and $B = T \restriction \ker(\Gamma_1)$. Assume

$$(A - \mu I_{\mathcal{H}})^{-1} \geq (B - \mu I_{\mathcal{H}})^{-1} \text{ for some } \mu \in \rho(A) \cap \rho(B) \cap \mathbb{R},$$

$$\overline{\gamma(z_0)} \in \mathcal{B}_2(\mathcal{H}),\ M(z_1)^{-1}, M(z_2) \text{ bounded for some } z_0, z_1, z_2 \in \mathbb{C}\backslash\mathbb{R}.$$

Then,

- $(B - zI_{\mathcal{H}})^{-1} - (A - zI_{\mathcal{H}})^{-1} = -\gamma(z)M(z)^{-1}\gamma(\bar{z})^* \in \mathcal{B}_1(\mathcal{H})$,
- $\operatorname{Im}(\log(\overline{M(z)}) \in \mathcal{B}_1(\mathcal{G})$ for all $z \in \mathbb{C}\backslash\mathbb{R}$,

  and

$$\xi(\lambda; B, A) = \lim_{\varepsilon \downarrow 0} \pi^{-1} \operatorname{tr}_{\mathcal{G}}\big(\operatorname{Im}\big(\log\big(\overline{M(\lambda + i\varepsilon)}\big)\big)\big) \text{ for a.e. } \lambda \in \mathbb{R},$$

  is the **spectral shift function** for the pair (B, A), in particular,

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

Main Abstract Result: Higher-Order Case

Theorem.

A, B self-adjoint, $S = A \cap B$ densely defined, and $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ a QBT,

$$A = T \restriction \ker(\Gamma_0) \text{ and } B = T \restriction \ker(\Gamma_1).$$

Assume

$$(A - \mu I_{\mathcal{H}})^{-1} \geq (B - \mu I_{\mathcal{H}})^{-1} \quad \text{for some } \mu \in \rho(A) \cap \rho(B) \cap \mathbb{R},$$

$$M(z_1)^{-1}, M(z_2) \text{ bounded for some } z_1, z_2 \in \mathbb{C} \backslash \mathbb{R},$$

and

$$\frac{d^p}{dz^p} \overline{\gamma(z)} \frac{d^q}{dz^q} \big(M(z)^{-1} \gamma(\bar{z})^* \big) \in \mathcal{B}_1(\mathcal{H}), \quad p + q = 2k,$$

$$\frac{d^q}{dz^q} \big(M(z)^{-1} \gamma(\bar{z})^* \big) \frac{d^p}{dz^p} \overline{\gamma(z)} \in \mathcal{B}_1(\mathcal{H}), \quad p + q = 2k,$$

$$\frac{d^j}{dz^j} \overline{M(z)} \in \mathcal{B}_{\frac{2k+1}{j}}(\mathcal{H}), \quad j = 1, \dots, 2k+1,$$

for some $k \in \mathbb{N}$.

Main Abstract Result: Higher-Order Case (contd.)

Theorem.

A, B self-adjoint, $S = A \cap B$ densely defined and $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ a QBT, $A = T \upharpoonright \ker(\Gamma_0)$ and $B = T \upharpoonright \ker(\Gamma_1)$. Assume

$$(A - \mu I_{\mathcal{H}})^{-1} \geq (B - \mu I_{\mathcal{H}})^{-1} \quad \text{for some } \mu \in \rho(A) \cap \rho(B) \cap \mathbb{R},$$

$$M(z_1)^{-1}, M(z_2) \text{ bounded for } z_1, z_2 \in \mathbb{C}\backslash\mathbb{R}, \text{ and } \mathcal{B}_p(\mathcal{G})\text{-conditions.}$$

Then,

- $\big[(B - zI_{\mathcal{H}})^{-(2k+1)} - (A - zI_{\mathcal{H}})^{-(2k+1)}\big] \in \mathcal{B}_1(\mathcal{H})$,
- $\operatorname{Im}\big(\log\big(\overline{M(\lambda)}\big)\big) \in \mathcal{B}_1(\mathcal{G})$ for all $z \in \mathbb{C}\backslash\mathbb{R}$,

and

$$\xi(\lambda; B, A) = \lim_{\varepsilon \downarrow 0} \pi^{-1} \operatorname{tr}\Big(\operatorname{Im}\big(\log\big(\overline{M(\lambda + i\varepsilon)}\big)\big)\Big) \text{ for a.e. } \lambda \in \mathbb{R},$$

is the **spectral shift function** for the pair (B, A), in particular,

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

Remarks:

- If A, B semibounded, $\mu < \inf(\sigma(A) \cup \sigma(B))$, then
$$(A - \mu I_{\mathcal{H}})^{-1} \geq (B - \mu I_{\mathcal{H}})^{-1} \quad \Longleftrightarrow \quad A \leq B$$
in accordance with $\xi(\lambda; B, A) = \pi^{-1}\mathrm{tr}_{\mathcal{G}}\big(\mathrm{Im}\big(\log\big(\overline{M(\lambda + i0)}\big)\big)\big) \geq 0$.
- Key difficulty: For $z \in \mathbb{C}^+$ prove that imaginary part of
$$\log\big(\overline{M(z)}\big) := -i\int_0^\infty \Big[\big(\overline{M(z)} + i\lambda\big)^{-1} - (1 + i\lambda)^{-1}\Big]\, d\lambda$$
is a trace class operator, Birman–Entina '67, Naboko '87, Carey '76, and G.–Makarov–Naboko '99.
Extend the exponential Nevanlinna–Herglotz representation
$$\log\big(\overline{M(z)}\big) = C + \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{t}{1 + \lambda^2}\right) \Xi(\lambda; B, A)\, d\lambda, \quad z \in \mathbb{C}^+,$$
on to the real line around μ.
- In Behrndt–Langer–Lotoreichik '13 for self-adjoint elliptic PDOs
$$\Big[(B - zI_{\mathcal{H}})^{-(2k+1)} - (A - zI_{\mathcal{H}})^{-(2k+1)}\Big] \in \mathcal{B}_1(\mathcal{H}), \quad z \in \rho(A) \cap \rho(B).$$

Remarks (contd.):

Representation of SSF via M-function:

- Rank 1, $k = 0$: **Langer–de Snoo–Yavrian '01**.
- Rank $n < \infty$, $k = 0$: **Behrndt–Malamud–Neidhardt '08**.
- Other representation via modified perturbation determinant for M for $k = 0$: **Malamud–Neidhardt '15**.

Representation of scattering matrix via M-function:

- Rank $n < \infty$: **Adamyan–Pavlov '86, Albeverio–Kurasov '00**, **Behrndt–Malamud–Neidhardt '08**.
- $k = 0$: **Behrndt–Malamud–Neidhardt '15, Mantile–Posilicano–Sini '15**.

Closely connected are

- **Mikhailova–Pavlov–Prokhorov**, *Intermediate Hamiltonian via Glazman's splitting and analytic perturbation for meromorphic matrix-functions*, Math. Nachr. **280**, 1376–1416 (2007).

Example 1: Robin boundary conditions

$$A_{\beta_0} f = -\Delta f + Vf, \quad \operatorname{dom}(A_{\beta_0}) = \big\{ f \in H^2(\Omega) : \beta_0 f|_{\partial\Omega} = \partial_\nu f|_{\partial\Omega} \big\},$$
$$A_{\beta_1} f = -\Delta f + Vf, \quad \operatorname{dom}(A_{\beta_1}) = \big\{ f \in H^2(\Omega) : \beta_1 f|_{\partial\Omega} = \partial_\nu f|_{\partial\Omega} \big\}.$$

- Ω domain in $\mathbb{R}^n$, $\partial\Omega$ smooth and compact;
- $V \in L^\infty(\Omega)$ real and $\beta_0, \beta_1 \in C^2(\partial\Omega)$ real, $\beta_0 \neq \beta_1$;
- **Neumann-to-Dirichlet map**: $\mathcal{N}(z) \partial_\nu f_z|_{\partial\Omega} = f_z|_{\partial\Omega}$ in $L^2(\partial\Omega)$.

Theorem.

For $k \geq (n-3)/4$ one has

- $(A_{\beta_1} - zI_{L^2(\Omega)})^{-(2k+1)} - (A_{\beta_0} - zI_{L^2(\Omega)})^{-(2k+1)} \in \mathcal{B}_1\big(L^2(\Omega)\big)$.
- **Spectral shift function** for the pair $(A_{\beta_1}, A_{\beta_0})$,

$$\xi(\lambda; A_{\beta_1}, A_{\beta_0}) = \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \operatorname{tr}_{L^2(\partial\Omega)} \Big(\operatorname{Im}\big(\log(\mathcal{M}_0(\lambda + i\varepsilon)) - \log(\mathcal{M}_1(\lambda + i\varepsilon))\big)\Big),$$

where $\mathcal{M}_j(z) = \frac{1}{\beta - \beta_j} \big(\beta_j \overline{\mathcal{N}(z)} - I_{L^2(\partial\Omega)}\big) \big(\beta \overline{\mathcal{N}(z)} - I_{L^2(\partial\Omega)}\big)^{-1}$, and $\beta \in \mathbb{R}$ such that $\beta_j(x) < \beta$ for all $x \in \partial\Omega$ and $j = 0, 1$.

Example 2: Compactly supported potentials in $\mathbb{R}^n$

- $A = -\Delta$ and $B = -\Delta + V$ with $\mathrm{dom}(A) = \mathrm{dom}(B) = H^2(\mathbb{R}^n)$
- $V \in L^\infty(\mathbb{R}^n)$ real-valued with compact support in $\mathcal{B}_+$

Multidimensional Glazman splitting: Instead of $\{A, B\}$ consider

$$\left\{A, \begin{pmatrix} A_+ & 0 \\ 0 & C \end{pmatrix}\right\}, \left\{\begin{pmatrix} A_+ & 0 \\ 0 & C \end{pmatrix}, \begin{pmatrix} B_+ & 0 \\ 0 & C \end{pmatrix}\right\}, \left\{\begin{pmatrix} B_+ & 0 \\ 0 & C \end{pmatrix}, B\right\},$$

where

$$L^2(\mathbb{R}^n) = L^2(\mathcal{B}_+) \oplus L^2(\mathcal{B}_+^c),$$

with $\mathcal{B}_+ \subset \mathbb{R}^n$ a fixed open ball and $\mathcal{S} = \partial\mathcal{B}_+$ the $(n-1)$-dimensional sphere, and

- $A_+ = -\Delta$ with $\mathrm{dom}(A_+) = H^2(\mathcal{B}_+) \cap H_0^1(\mathcal{B}_+)$ in $L^2(\mathcal{B}_+)$;
- $B_+ = -\Delta + V$ with $\mathrm{dom}(B_+) = H^2(\mathcal{B}_+) \cap H_0^1(\mathcal{B}_+)$ in $L^2(\mathcal{B}_+)$;
- $C = -\Delta$ with $\mathrm{dom}(C) = H^2(\mathcal{B}_+^c) \cap H_0^1(\mathcal{B}_+^c)$ in $L^2(\mathcal{B}_+^c)$.

We recall: SSF for the pair (B_+, A_+) is $\xi(\lambda; B_+, A_+) = N_{A_+}(\lambda) - N_{B_+}(\lambda)$, $\lambda \in \mathbb{R}$.

Example 2: Compactly supported potentials in $\mathbb{R}^n$ (contd.)

Theorem.

For $k > (n-2)/4$ one has

- $\big[(B - zI_{L^2(\mathbb{R}^n)})^{-(2k+1)} - (A - zI_{L^2(\mathbb{R}^n)})^{-(2k+1)}\big] \in \mathcal{B}_1\big(L^2(\mathbb{R}^n)\big)$.
- **Spectral shift function** for the pair $(B = -\Delta + V, A = -\Delta)$,

$$\begin{aligned}\xi(\lambda; B, A) = \lim_{\varepsilon \downarrow 0} \pi^{-1} \operatorname{tr}_{L^2(\mathcal{B}_+)}\Big(\operatorname{Im}\big(\log(\mathfrak{N}(\lambda + i0)) - \log(\mathfrak{N}_V(\lambda + i0))\big)\Big)\\ + N_{A_+}(\lambda) - N_{B_+}(\lambda),\end{aligned}$$

where

$$\mathfrak{N}(z) = \imath\big(\mathcal{D}_+(z) + \mathcal{D}_-(z)\big)^{-1}\widetilde{\imath} \colon L^2(\partial\mathcal{B}_+) \to L^2(\partial\mathcal{B}_+),$$
$$\mathfrak{N}_V(z) = \imath\big(\mathcal{D}_+^V(z) + \mathcal{D}_-(z)\big)^{-1}\widetilde{\imath} \colon L^2(\partial\mathcal{B}_+) \to L^2(\partial\mathcal{B}_+),$$

and $\mathcal{D}_\pm(z)$ and $\mathcal{D}_+^V(z)$ Dirichlet-to-Neumann maps for $-\Delta - zI$ and $-\Delta + V - zI$ on $\mathcal{B}_+$ and $\mathcal{B}_+^c$.

Example 2: Compactly supported potentials in $\mathbb{R}^n$ (contd.)

Here $\imath$ is a uniformly positive self-adjoint operator in $L^2(\mathcal{S})$ defined on the dense subspace $H^{1/2}(\mathcal{S})$ (and $\imath$ is regarded as an isomorphism from $H^{1/2}(\mathcal{S})$ onto $L^2(\mathcal{S})$), and $\widetilde{\imath^{-1}}$ is the extension of $\imath^{-1}$ to an isomorphism from $H^{-1/2}(\mathcal{S})$ onto $L^2(\mathcal{S})$. A typical and convenient choice for $\imath$ is $(-\Delta_{\mathcal{S}} + I_{L^2(\mathcal{S})})^{1/4}$, where $-\Delta_{\mathcal{S}}$ is the Laplace–Beltrami operator on the sphere $\mathcal{S}$.

Note. $\xi(\,\cdot\,; B, A)$ is continuous for $\lambda \geq 0$, although $N_{A_+} - N_{B_+}$ is a step function.