Spectral Shift Functions and Dirichlet-to-Neumann Maps

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Topics discussed:

- A warm up: **Self-adjoint extensions**, **Krein-type resolvent formulas** for $1d$ Schrödinger operators
- **Resolvent trace formulas.**
- **Krein–Lifshitz spectral shift (SSF) functions.**
- Hints at an extension of **SSF**, the **Spectral Shift Operator (SSO)**, whose **trace** equals **SSF**.
- Connect **SSO** with **abstract Weyl–Titchmarsh M-operators**.
- Sketch **applications** of **Dirichlet-to-Neumann maps**, more generally, **abstract Weyl–Titchmarsh M-operators**, to **PDEs**.

Some Literature:

In the 1d context:

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).

In the Abstract and PDE context:

F.G., K. A. Makarov, and S. N. Naboko, *The spectral shift operator*, in *Mathematical Results in Quantum Mechanics*, J. Dittrich, P. Exner, and M. Tater (eds.), Operator Theory: Advances and Applications, Vol. 108, Birkhäuser, Basel, 1999, pp. 59–90.

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

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 the following.

A Bit of Notation (contd.):

- If A is closable in $\mathcal{H}$, then $\overline{A}$ denotes the **operator closure** of A in $\mathcal{H}$.

- $\mathcal{B}(\mathcal{H})$ 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 $A \in \mathcal{B}_1(\mathcal{H})$.

Maximal and Minimal Schrödinger Operators in 1d

We'll use the 1d case of Schrödinger operators as a warm up case: 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

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

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

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

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

$$H_{\theta_0,\theta_R} f = \tau f, \quad \theta_0, \theta_R \in [0,\pi), \quad \textbf{separated b.c.'s,}$$
$$f \in \operatorname{dom}(H_{\theta_0,\theta_R}) = \big\{ g \in \operatorname{dom}(H_{\max}) \,\big|\, \cos(\theta_0) g(0) + \sin(\theta_0) g'(0) = 0, \\ \cos(\theta_R) g(R) - \sin(\theta_R) g'(R) = 0 \big\}$$

and

$$H_{K,\phi} f = \tau f, \quad \phi \in [0,2\pi), \; K \in \mathrm{SL}(2,\mathbb{R}), \quad \textbf{coupled b.c.'s,}$$
$$f \in \operatorname{dom}(H_{K,\phi}) = \left\{ g \in \operatorname{dom}(H_{\max}) \,\middle|\, \begin{pmatrix} g(R) \\ g'(R) \end{pmatrix} = e^{i\phi} K \begin{pmatrix} g(0) \\ g'(0) \end{pmatrix} \right\}.$$

$\mathrm{SL}(2,\mathbb{R})$ 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.)

Indeed, one can unify separated and coupled boundary conditions as follows:

Theorem.

The operator $H_{F,G}$,

$$H_{F,G} f = \tau f, \; f \in \operatorname{dom}(H_{F,G}) = \left\{ g \in \operatorname{dom}(H_{\max}) \,\middle|\, F \begin{pmatrix} g(0) \\ g'(0) \end{pmatrix} = G \begin{pmatrix} g(R) \\ g'(R) \end{pmatrix} \right\},$$

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

In particular, the case of separated boundary conditions corresponds to

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

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

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

The Basics of Boundary Data Maps

Boundary Data Maps:

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

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

Then,

$$\gamma_{F,G} = D_{F,G}\gamma_D + N_{F,G}\gamma_N, \quad D_{F,G} = \begin{pmatrix} F_{1,1} & -G_{1,1} \\ F_{2,1} & -G_{2,1} \end{pmatrix}, \; N_{F,G} = \begin{pmatrix} F_{1,2} & G_{1,2} \\ F_{2,2} & G_{2,2} \end{pmatrix},$$

where γ_D and γ_N represent **Dirichlet** and **Neumann traces**,

$$\gamma_D u = \begin{pmatrix} u(0) \\ u(R) \end{pmatrix}, \quad \gamma_N u = \begin{pmatrix} -u'(0) \\ u'(R) \end{pmatrix}.$$

Moreover, define

$$S_{F',G',F,G} = N_{F',G'} D^*_{F,G} - D_{F',G'} N^*_{F,G}.$$

The Basics of Boundary Data Maps (contd.)

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

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

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

Let $F, G, F', G' \in \mathbb{C}^{2\times 2}$ with F, G satisfying $\operatorname{rank}(F \quad G) = 2$, $FJF^* = GJG^*$, $J = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$, and similarly for F', G'. Assuming $z \in \rho(H_{F,G})$, we introduce the **boundary data map** (an **extension** of **Dirichlet-to Neumann** and **Robin-to-Robin maps**) by

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

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

The Basics of Boundary Data Maps (contd.)

Basic Properties of $\Lambda_{F,G}^{F',G'}(z)$:

$$\Lambda_{F,G}^{F',G'}(z) = D_{F',G'}\Lambda_{F,G}^{D}(z) + N_{F',G'}\Lambda_{F,G}^{N}(z), \quad z \in \rho(H_{F,G}),$$

$$\Lambda_{F,G}^{F,G}(z) = I_2, \quad z \in \rho(H_{F,G}),$$

$$\Lambda_{F',G'}^{F'',G''}(z)\,\Lambda_{F,G}^{F',G'}(z) = \Lambda_{F,G}^{F'',G''}(z), \quad z \in \rho(H_{F,G}) \cap \rho(H_{F',G'}),$$

$$\Lambda_{F,G}^{F',G'}(z) = \left[\Lambda_{F',G'}^{F,G}(z)\right]^{-1}, \quad z \in \rho(H_{F,G}) \cap \rho(H_{F',G'}).$$

Resolvent Connection:

Theorem.

Let $F, G, F', G' \in \mathbb{C}^{2\times 2}$ with F, G satisfying $\operatorname{rank}(F \quad G) = 2$, $FJF^* = GJG^*$, $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, and similarly for F', G'.

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

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

BD Maps and Krein's Resolvent Formula Revisited

Theorem.

Let $F, G \in \mathbb{C}^{2\times 2}$ and $F', G' \in \mathbb{C}^{2\times 2}$ satisfy $\operatorname{rank}(F \quad G) = 2$, $FJF^* = GJG^*$, $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, and similarly for F', G', and let $z \in \rho(H_{F,G}) \cap \rho(H_{F',G'})$.

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

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

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

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

where

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

BD Maps, Fredholm Dets., and Trace Formulas

The connection between **BD maps and trace formulas:**

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

Theorem.

Let $F, G \in \mathbb{C}^{2\times 2}$ and $F', G' \in \mathbb{C}^{2\times 2}$ satisfy $\operatorname{rank}(F \;\; G) = 2$, $FJF^* = GJG^*$, $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, and similarly for F', G'. Then, for $z \in \mathbb{C}\backslash[e_0, \infty)$,

$$\operatorname{tr}_{L^2((0,R);dx)}\big((H_{F',G'} - z)^{-1} - (H_{F,G} - z)^{-1}\big) = -\frac{d}{dz} \ln\Big(\det_{\mathbb{C}^2}\Big(\Lambda_{F,G}^{F',G'}(z)\Big)\Big).$$

Perhaps, one of the most compelling reasons to study $\Lambda_{F,G}^{F',G'}(z)$ ....

Note. $\Lambda_{F,G}^{F',G'}(z)$ is quite different from the underlying 2×2 matrix-valued **Weyl–Titchmarsh function**, though, both are **Nevanlinna–Herglotz functions**.

BD Maps and Spectral Shift Functions

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

We will soon review basic properties of spectral shift functions!

Using the standard normalization,

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

Krein's trace formula reads

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

where

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

BD Maps and Spectral Shift Functions (contd.)

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

Theorem.

Let $F, G \in \mathbb{C}^{2\times 2}$ and $F', G' \in \mathbb{C}^{2\times 2}$ satisfy $\operatorname{rank}(F \;\; G) = 2$, $FJF^* = GJG^*$, $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, and similarly for F', G'. Then, for a.e. $\lambda \in \mathbb{R}$,

$$\boxed{\xi(\lambda; H_{F',G'}, H_{F,G}) = \pi^{-1} \lim_{\varepsilon \downarrow 0} \operatorname{Im}\Big(\ln\Big(\eta_{F',G',F,G} \det_{\mathbb{C}^2}\Big(\Lambda_{F,G}^{F',G'}(\lambda + i\varepsilon)\Big)\Big)\Big),}$$

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

A quick SSF Summary:

Here comes the promised summary on basic properties of **Spectral Shift Functions (SSF)**:

General Hypothesis.

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

I. M. Lifshitz, 1952.

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

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

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 there 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

$$\xi(b_-; B, A) - \xi(a_+; B, A) = \dim(\operatorname{ran}(E_B(\delta))) - \dim(\operatorname{ran}(E_A(\delta))).$$

- There is also a 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 there 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 are discussed in **V. Peller '85** (he employs Besov spaces).

Birman–Krein formula.

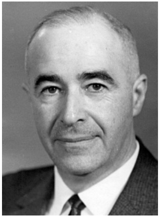
Assume $(*)$. The scattering matrix $\{S(\lambda; B, A)\}_{\lambda \in \sigma_{ac}(A)}$ for the pair (B, A) satisfies

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

The Krein–Lifshitz spectral shift function ξ:

"On the shoulders of giants":

Ilya Mikhailovich Lifshitz (January 13, 1917 – October 23, 1982):



Well-known Theoretical Physicist: Worked in solid state physics, electron theory of metals, disordered systems, Lifshitz tails, Lifshitz singularity, the theory of polymers; **introduced the concept of the spectral shift function for finite-rank perturbations in 1952.**

Mark Grigorievich Krein (April 3, 1907 – October 17, 1989):

Mathematician Extraordinaire: One of the giants of 20th century mathematics, Wolf Prize in Mathematics in 1982; **introduced the theory of the spectral shift function in the period of 1953–1963.**

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

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

SSF: Generalizations contd.

D. R. Yafaev '05.

Assume that for some odd, $m \in \mathbb{N}$,

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

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

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

Note. Yafaev assumes **no** spectral gaps of A ($\longrightarrow$ applicable to **massless** Dirac-type operators, prime examples of **non-Fredholm model operators**, with applications to **graphene** ....).

SSF and Quasi Boundary Triples: A Quick Overview

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

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

Next, introduce T such that

$$S \subsetneqq A, B \subsetneqq T \subseteq S^*, \ \text{ s.t. } \ \overline{T} = S^*,$$

and boundary maps $\Gamma_0, \Gamma_1 \colon \mathrm{dom}(T) \to \mathcal{G}$ ($\mathcal{G}$ an auxiliary Hilbert space) such that

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

The triple, $(\mathcal{G}, \Gamma_0, \Gamma_1)$, is called a **Quasi Boundary Triple (QBT)**.

In addition we need the **γ-field** and abstract **Weyl–Titchmarsh** fct. $M(\,\cdot\,)$: Let $f_z \in \ker(T - zI_{\mathcal{H}})$, $\ z \in \mathbb{C}\backslash\mathbb{R}$,

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

$$M(z) : \mathrm{ran}(\Gamma_0) \to \mathrm{ran}(\Gamma_1), \quad \Gamma_0 f_z \mapsto \Gamma_1 f_z, \quad z \in \mathbb{C}\backslash\mathbb{R}, \ \text{(closable)}.$$

Then a **Krein-type resolvent formula** holds

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

SSF and QBT: A Quick Overview (contd.)

Fact. If $M(\,\cdot\,) \in \mathcal{B}(\mathcal{G})$ is a bounded **Nevanlinna–Herglotz** fct. (i.e., $M(\,\cdot\,)$ is analytic on $\mathbb{C}_+$ and $\mathrm{Im}(M(z)) \geq 0$, $z \in \mathbb{C}_+$) s.t. $M(\,\cdot\,)^{-1} \in \mathcal{B}(\mathcal{G})$ is bounded, then also $\log(M(\,\cdot\,))$ is a bounded **Nevanlinna–Herglotz** fct. with representation

$$\log\big(\overline{M(z)}\big) = \mathrm{Re}\big(\log\big(\overline{M(i)}\big)\big) + \int_{\mathbb{R}} \bigg(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\bigg)\, \Xi(\lambda; B, A)\, d\lambda, \quad z \in \mathbb{C}_+,$$

with $0 \leq \Xi(\lambda; B, A) \leq I_{\mathcal{G}}$. Next, suppose that for some $k \in \mathbb{N}_0$,

$$\big[(B - zI_{\mathcal{H}})^{-(2k+1)} - (A - zI_{\mathcal{H}})^{-(2k+1)}\big] \in \mathcal{B}_1(\mathcal{H}), \quad z \in \mathbb{C}\backslash\mathbb{R},$$

then

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

where, for a.e. $\lambda \in \mathbb{R}$, $\xi(\,\cdot\,, B, A)$ is the Spectral Shift Function (SSF)

$$\xi(\lambda; B, A) = \mathrm{tr}_{\mathcal{G}}(\Xi(\lambda; B, A)) = \pi^{-1} \sum_{j \in J} \lim_{\varepsilon \downarrow 0} \big(\mathrm{Im}(\log(M(\lambda + i\varepsilon))\varphi_j, \varphi_j\big)_{\mathcal{G}}.$$

Here $\{\varphi_j\}_{j \in J}$ is an ONB in $\mathcal{G}$. For $k = 0$ this simplifies to

$$\xi(\lambda; B, A) = \mathrm{tr}_{\mathcal{G}}(\Xi(\lambda; B, A)) = \pi^{-1} \lim_{\varepsilon \downarrow 0} \mathrm{tr}_{\mathcal{G}}\big(\mathrm{Im}(\log(M(\lambda + i\varepsilon)))\big).$$

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
$S \subset T \subset \overline{T} = S^*$ 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) $\Gamma := \binom{\Gamma_0}{\Gamma_1} : \mathrm{dom}(T) \to \mathcal{G} \times \mathcal{G}$ dense range.

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

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

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

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

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

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.,

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

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

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

and

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

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

Note. In this scheme, $S = T \upharpoonright \{\ker(\Gamma_0) \cap \ker(\Gamma_1)\}$.

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, $A = T \upharpoonright \ker(\Gamma_0)$, and $B = T \upharpoonright \ker(\Gamma_1)$. Assume

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

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

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

$$\boxed{\xi(\lambda; B, A) = \operatorname{tr}_{\mathcal{G}}(\Xi(\lambda; B, A)) = \pi^{-1} \lim_{\varepsilon \downarrow 0} \operatorname{tr}_{\mathcal{G}}\big(\operatorname{Im}\big(\log\big(\overline{M(\lambda + i\varepsilon)}\big)\big)\big),}$$

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,

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

Assume

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

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

and

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

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

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

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

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

Theorem (cont.).

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

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

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

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 for a.e. $\lambda \in \mathbb{R}$ (and with $\{\varphi_j\}_{j\in J}$ an ONB in $\mathcal{G}$),

$$\xi(\lambda; B, A) = \operatorname{tr}_{\mathcal{G}}(\Xi(\lambda; B, A)) = \pi^{-1} \sum_{j\in J} \lim_{\varepsilon\downarrow 0}\big(\operatorname{Im}\big(\log\big(\overline{M(\lambda + i\varepsilon)}\varphi_j, \varphi_j\big)_{\mathcal{G}}$$

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

$$\log\big(\overline{M(z)}\big) := -i \int_0^\infty \Big[\big(\overline{M(z)} + i\lambda I_{\mathcal{G}}\big)^{-1} - (1 + i\lambda)^{-1} I_{\mathcal{G}}\Big]\, d\lambda$$

is a trace class operator, Birman–Entina ’67, Naboko ’87, Carey ’76, G.–Makarov–Naboko ’99, and G.–Makarov ’00.

Exploit the **exponential Nevanlinna–Herglotz representation**

$$\log\big(\overline{M(z)}\big) = C + \int_{\mathbb{R}} \bigg(\frac{1}{\lambda - z} - \frac{\lambda}{1 + \lambda^2}\bigg) \Xi(\lambda; B, A)\, d\lambda, \quad z \in \mathbb{C}_+,$$

with $C = C^* \in \mathcal{B}(\mathcal{G})$, $0 \leq \Xi(\lambda; B, A) \leq I_{\mathcal{G}}$, $\xi(\lambda; B, A) = \mathrm{tr}_{\mathcal{G}}(\Xi(\lambda; B, A))$, etc.

Remarks (contd.):

- In **Behrndt–Langer–Lotoreichik '13** for self-adjoint elliptic PDOs

$$\big[(B - zI_{\mathcal{H}})^{-(2k+1)} - (A - zI_{\mathcal{H}})^{-(2k+1)}\big] \in \mathcal{B}_1(\mathcal{H}), \quad z \in \rho(A) \cap \rho(B).$$

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).

An Extension of the Abstract Result

The condition

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

can be inconvenient for certain PDE applications. Here is a slight variant of this: Suppose that there exists a self-adjoint operator C in $\mathcal{H}$ such that

$$(C-\zeta_A I_{\mathcal{H}})^{-1} \geq (A-\zeta_A I_{\mathcal{H}})^{-1} \text{ and } (C-\zeta_B I_{\mathcal{H}})^{-1} \geq (B-\zeta_B I_{\mathcal{H}})^{-1}$$

for some $\zeta_A \in \rho(A) \cap \rho(C) \cap \mathbb{R}$ and some $\zeta_B \in \rho(B) \cap \rho(C) \cap \mathbb{R}$. In addition, assume that the closed symmetric operators $S_A = A \cap C$ and $S_B = B \cap C$ are both densely defined and choose quasi boundary triples $\{\mathcal{G}_A, \Gamma_0^A, \Gamma_1^A\}$ and $\{\mathcal{G}_B, \Gamma_0^B, \Gamma_1^B\}$ with γ-fields γ_A, γ_B and Weyl functions M_A, M_B for

$$T_A = {S_A}^* \restriction \big(\text{dom}(A) + \text{dom}(C)\big) \text{ and } T_B = {S_B}^* \restriction \big(\text{dom}(B) + \text{dom}(C)\big)$$

such that

$$C = T_A \restriction \ker\big(\Gamma_0^A\big) = T_B \restriction \ker\big(\Gamma_0^B\big),$$

and

$$A = T_A \restriction \ker\big(\Gamma_1^A\big) \text{ and } B = T_B \restriction \ker\big(\Gamma_1^B\big),$$

An Extension of the Abstract Result (contd.)

Finally, assume that for some $k \in \mathbb{N}_0$, all the previous $\mathcal{B}_p$-conditions are satisfied for the γ-fields γ_A, γ_B and the Weyl functions M_A, M_B. Then the difference of the $2k+1$-th powers of the resolvents of A and C, and the difference of the $2k+1$-th powers of the resolvents of B and C are trace class operators, and for orthonormal bases $(\varphi_j)_{j \in J}$ in $\mathcal{G}_A$ and $(\psi_\ell)_{\ell \in L}$ in $\mathcal{G}_B$ ($J, L \subseteq \mathbb{N}$ appropriate index sets),

$$\xi_A(\lambda; C, A) = \pi^{-1} \sum_{j \in J} \lim_{\varepsilon \downarrow 0} \big(\text{Im}\big(\log\big(\overline{M_A(\lambda + i\varepsilon)}\big)\big)\varphi_j, \varphi_j\big)_{\mathcal{G}_A} \text{ for a.e. } \lambda \in \mathbb{R},$$

and

$$\xi_B(\lambda; C, B) = \pi^{-1} \sum_{\ell \in L} \lim_{\varepsilon \downarrow 0} \big(\text{Im}\big(\log\big(\overline{M_B(\lambda + i\varepsilon)}\big)\big)\psi_\ell, \psi_\ell\big)_{\mathcal{G}_B} \text{ for a.e. } \lambda \in \mathbb{R},$$

are spectral shift functions for the pairs $\{C, A\}$ and $\{C, B\}$.

An Extension of the Abstract Result (contd.)

It follows that for $z \in \rho(A) \cap \rho(B) \cap \rho(C)$,

$$\begin{aligned}
&\operatorname{tr}_{\mathcal{H}} \big((B - zI_{\mathcal{H}})^{-(2k+1)} - (A - zI_{\mathcal{H}})^{-(2k+1)}\big) \\
&\quad = \operatorname{tr}_{\mathcal{H}}\big((B - zI_{\mathcal{H}})^{-(2k+1)} - (C - zI_{\mathcal{H}})^{-(2k+1)}\big) \\
&\qquad - \operatorname{tr}_{\mathcal{H}}\big((A - zI_{\mathcal{H}})^{-(2k+1)} - (C - zI_{\mathcal{H}})^{-(2k+1)}\big) \\
&\quad = -(2k+1) \int_{\mathbb{R}} \frac{[\xi_B(\lambda : C, B) - \xi_A(\lambda; C, A)]\, d\lambda}{(\lambda - z)^{2k+2}}
\end{aligned}$$

and

$$\int_{\mathbb{R}} \frac{|\xi_B(\lambda; C, B) - \xi_A(\lambda; C, A)|\, d\lambda}{(1 + |\lambda|)^{2m+2}} < \infty.$$

Therefore,

$$\xi(\lambda; A, B) = \xi_B(\lambda; C, B) - \xi_A(\lambda; C, A) \text{ for a.e. } \lambda \in \mathbb{R},$$

is a spectral shift function for the pair $\{A, B\}$.

Example 1: Robin boundary conditions

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

- 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 $(A_{\beta_1}, A_{\beta_0})$,

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

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

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

We recall: SSF for the pair (B_+, A_+) is $\xi(\lambda; B_+, A_+) = N_{A_+}(\lambda) - N_{B_+}(\lambda)$, $\lambda \in \mathbb{R}$, i.e., a difference of **eigenvalue counting functions**.

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 $(B = -\Delta + V, A = -\Delta)$,

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

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 $\mathcal{B}_+^c$; $\imath, \widetilde{\imath}$ are appropriate isomorphisms, e.g., $\imath = (-\Delta_{\mathcal{S}} + I_{L^2(\mathcal{S})})^{1/4}$, with $-\Delta_{\mathcal{S}}$ the Laplace–Beltrami operator on the sphere $\mathcal{S} = \partial\mathcal{B}_+$ .....

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