Applications of Spectral Shift Functions. I: Basic Properties of SSFs

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A Classic Problem in Operator Theory:

- **Perturbation Theory**
- **Spectral Theory**

More precisely, suppose we are given an unperturbed operator H_0, and an **additive perturbation** V, consider $H = H_0 + V$.

Basic Problem of (Perturbative) Spectral Theory: Given spectral properties of the unperturbed operator H_0, determine spectral properties of H.

(This is a fundamental problem, but one that's a lot easier formulated than solved!)

Standard Example: Two-Body Quantum Mechanics

H_0 models kinetic energy

V models potential energy

$H = H_0 + V$ represents the total Hamiltonian

A Classic Problem in Operator Theory (contd.):

Spectral Theory: Typically is divided into two parts:

(*i*) **A study of the discrete spectrum:** Searching for **eigenvalues** (think **bound states** in quantum systems).

(*ii*) **A study of the (absolutely) continuous spectrum:** Leading toward **scattering theory** (think **scattering amplitudes, cross sections,** etc.).

There are also **eigenvalues embedded in the continuous spectrum**, but that's for another day.

Today, **spectral theory** is a vast area in operator theory! We will just scratch a bit at its surface in these lectures.

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

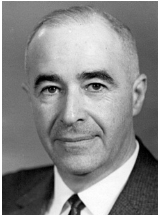
- $\det_{\mathcal{H}}(I_{\mathcal{H}} - A) = \prod_{j\in\mathcal{J}}[1 - \lambda_j(A)]$ denotes the **Fredholm determinant**, defined for $A \in \mathcal{B}_1(\mathcal{H})$.

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

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 rank one 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.**

A Short Course on the Spectral Shift Function ξ:

Given two **self-adjoint** operators H, H_0 in $\mathcal{H}$, think of H as an additive perturbation of H_0 by the operator V, that is,

$$H = H_0 \text{ ``}+\text{'' } V.$$

We assume that the "perturbation" $V = H - H_0$ satisfies one of the following:

- **Trace class perturbations:** $V = \overline{[H - H_0]} \in \mathcal{B}_1(\mathcal{H})$.
- **Relative trace class:** $V(H_0 - z\, I_{\mathcal{H}})^{-1} \in \mathcal{B}_1(\mathcal{H})$ for some (hence, all) $z \in \mathbb{C}\backslash\mathbb{R}$.
- **Resolvent comparable:** $\big[(H - z\, I_{\mathcal{H}})^{-1} - (H_0 - z\, I_{\mathcal{H}})^{-1}\big] \in \mathcal{B}_1(\mathcal{H})$.

Perhaps, the best way to formally introduce the **Krein–Lifshitz spectral shift function** $\xi(\,\cdot\,; H, H_0)$ is to show what it can do: It computes **traces**!

More precisely, the spectral shift function (SSF) is a real-valued function on $\mathbb{R}$ that satisfies the **trace formula**

$$\boxed{\operatorname{tr}_{\mathcal{H}}(f(H) - f(H_0)) = \int_{\mathbb{R}} f'(\lambda)\, \xi(\lambda; H, H_0)\, d\lambda,}$$

for "appropriate" functions f.

A Short Course on the SSF ξ (contd.):

For example, take the resolvent function $(\cdot - z)^{-1}$, $z \in \mathbb{C}\backslash\mathbb{R}$,

$$\operatorname{tr}_{\mathcal{H}}\big((H - z\,I_{\mathcal{H}})^{-1} - (H_0 - z\,I_{\mathcal{H}})^{-1}\big) = -\int_{\mathbb{R}} \frac{\xi(\lambda; H, H_0)\,d\lambda}{(\lambda - z)^2}, \quad z \in \mathbb{C}\backslash\mathbb{R},$$

or the exponential function $e^{-t\,\cdot}$, $t > 0$, assuming H_0, H to be bounded from below, $H_0 \geq cI_{\mathcal{H}}$ for some $c \in \mathbb{R}$,

$$\operatorname{tr}_{\mathcal{H}}\big(e^{-tH} - e^{-tH_0}\big) = -t\int_{[c,\infty)} e^{-t\lambda}\xi(\lambda; H, H_0)\,d\lambda, \quad t > 0.$$

Here $c = \min\{\inf(\sigma(H)), \inf(\sigma(H_0))\}$.

The general trace formula works, e.g., for $f \in C^1(\mathbb{R})$ with $f'(\lambda) = \int_{\mathbb{R}} e^{-i\lambda s} d\sigma(s)$ and $d\sigma$ a finite signed measure;

$f(\lambda) = (\lambda - z)^{-1}$;

or, $\widehat{f} \in L^1(\mathbb{R}; (1 + |p|)dp)$ (implies $f \in C^1(\mathbb{R})$), etc.

V. Peller has necessary conditions on f, and also sufficient conditions on f in terms of certain Besov spaces. These spaces are not that far apart ....

Possible Applications:

- **Spectral Theory** (eigenvalue counting functions, inverse spectral problems, trace formulas, spectral averaging, localization for random Hamiltonians, etc.)
- **Scattering Theory** (sum rules, such as Levinson's Theorem, time delay, fixed energy scattering matrices, etc.)
- **Quantum Mechanics** (Solid State Physics: Friedel's sum rule, etc.)
- **Statistical Mechanics** (convexity of trace functionals, density-functional theory, density matrices, etc.).
- **Index Theory** (Fredholm and Witten indices.)
- Almost everywhere where traces and/or determinants involving **pairs of self-adjoint operators** are relevant.

The Spectral Shift Function ξ: Examples

We start with some **Examples**:

Here's a **non-serious** one:

- $H, H_0 \in \mathbb{R}$ (really, a joke!), the trace formula then becomes the **Newton–Leibniz "trace" formula**, a.k.a., **the fundamental theorem of calculus (FTC)**:

$$f(H) - f(H_0) = \int_{[H_0, H]} f'(\lambda)\, d\lambda$$

and thus,

$$\xi(\cdot\,; H, H_0) = \chi_{[H_0,H]}(\cdot) = \text{characteristic function of the interval } [H_0, H].$$

The Spectral Shift Function ξ: Examples (contd.)

For our next example, the **finite-dimensional case**, we first recall the spectral theorem for **self-adjoint** matrices $A = A^*$ in $\mathbb{C}^n$:

Let $\sigma(A) = \{\lambda_j(A)\}_{1 \leq j \leq m}$, $m \leq n$, be the eigenvalues of A, and denote by $P_j(A)$ the associated projection onto the eigenspace corresponding to $\lambda_j(A)$, $1 \leq j \leq m$. Then

$$A = \sum_{j=1}^{m} \lambda_j(A) P_j(A), \quad P_j(A) = \sum_{k=1}^{m_j} (\,\cdot\,, f_{j,k})_{\mathbb{C}^n} f_{j,k},$$

where $(f_{j,k}, f_{j,\ell})_{\mathbb{C}^n} = \delta_{k,\ell}$, $1 \leq k, \ell \leq m_j$, with m_j the multiplicity of the eigenvalue $\lambda_j(A)$ of A. Introducing

$$E_A((-\infty, \lambda]) = \sum_{j \text{ s.t. } \lambda_j(A) \leq \lambda} P_j(A), \quad \lambda \in \mathbb{R},$$

then (employing the Stieltjes integral)

$$A = \sum_{j=1}^{m} \lambda_j(A) P_j(A) = \int_{\mathbb{R}} \lambda \, dE_A(\lambda), \quad f(A) = \sum_{j=1}^{m} f(\lambda_j(A)) P_j(A) = \int_{\mathbb{R}} f(\lambda) \, dE_A(\lambda)$$

for bounded measurable functions f on $\mathbb{R}$.

The Spectral Shift Function ξ: Examples (contd.)

- H, H_0 **self-adjoint** matrices in $\mathbb{C}^n$ (**I. M. Lifshitz trace formula**):

$$\operatorname{tr}_{\mathbb{C}^n}(f(H) - f(H_0)) = \operatorname{tr}_{\mathbb{C}^n}\bigg(\int_{\mathbb{R}} f(\lambda) dE_H(\lambda) - \int_{\mathbb{R}} f(\lambda) dE_{H_0}(\lambda)\bigg)$$

$$= \operatorname{tr}_{\mathbb{C}^n}\bigg(\int_{\mathbb{R}} f(\lambda) d(E_H(\lambda) - E_{H_0}(\lambda))\bigg) = \int_{\mathbb{R}} f(\lambda) d\operatorname{tr}_{\mathbb{C}^n}(E_H(\lambda) - E_{H_0}(\lambda))$$

$$= -\int_{\mathbb{R}} f'(\lambda) \operatorname{tr}_{\mathbb{C}^n}(E_H(\lambda) - E_{H_0}(\lambda)) d\lambda$$

implies

$$\xi(\lambda; H, H_0) = -\operatorname{tr}_{\mathbb{C}^n}(E_H(\lambda) - E_{H_0}(\lambda)), \quad \lambda \in \mathbb{R}.$$

WARNING: Generally, $\xi(\,\cdot\,; H, H_0) = -\operatorname{tr}_{\mathcal{H}}(E_H(\cdot) - E_{H_0}(\cdot))$ is **NOT** correct if $\dim(\mathcal{H}) = \infty$!

M. Krein constructed a simple example where $[E_H(\cdot) - E_{H_0}(\cdot)]$ is **NOT** necessarily of trace class even for $V = [H - H_0]$ of rank one! (He used half-line Laplacians with different boundary conditions.)

A Short Course on the SSF ξ (contd.):

Recall the **Trace** and the **Determinant:** Let $\lambda_j(T)$, $j \in \mathcal{J}$ ($\mathcal{J} \subseteq \mathbb{N}$ an index set) denote the eigenvalues of $T \in \mathcal{B}_\infty(\mathcal{H})$, counting algebraic multiplicity.

$K \in \mathcal{B}_1(\mathcal{H})$, then $\sum_{j\in\mathcal{J}} \lambda_j\big((K^*K)^{1/2}\big) < \infty$ and

$$\mathrm{tr}_{\mathcal{H}}(K) = \sum_{j\in\mathcal{J}} \lambda_j(K), \qquad \det_{\mathcal{H}}(I_{\mathcal{H}} - K) = \prod_{j\in\mathcal{J}} [1 - \lambda_j(K)].$$

The **Perturbation Determinant:** H and H_0 self-adjoint in $\mathcal{H}$, $\quad H = H_0 + V$,

$$D_{H/H_0}(z) = \det_{\mathcal{H}}\big((H - z\,I_{\mathcal{H}})(H_0 - z\,I_{\mathcal{H}})^{-1}\big) = \det_{\mathcal{H}}\big(I_{\mathcal{H}} + V(H_0 - z\,I_{\mathcal{H}})^{-1}\big).$$

In the **matrix** case, view $D_{H/H_0}(z)$ as the quotient

$$D_{H/H_0}(z) = \frac{\det_{\mathcal{H}}(H - z\,I_{\mathcal{H}})}{\det_{\mathcal{H}}(H_0 - z\,I_{\mathcal{H}})}.$$

Example. If $H_0 = -(d^2/dx^2)$, $\quad H = -(d^2/dx^2) + V(\cdot)$ in $L^2(\mathbb{R}; dx)$, $V \in L^1(\mathbb{R}; (1+|x|)dx)$, real-valued, then

$$D_{H/H_0}(z) = \textbf{Jost} \text{ function} = \textbf{Evans} \text{ function}.$$

A Short Course on the SSF ξ (contd.):

The general **Krein trace formula** for the trace class perturbations V, i.e., $V = \overline{[H - H_0]} \in \mathcal{B}_1(\mathcal{H})$:

$$\xi(\lambda; H, H_0) = \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \operatorname{Im}(\ln(D_{H/H_0}(\lambda + i\varepsilon))) \text{ for a.e. } \lambda \in \mathbb{R}, \qquad (*)$$

where

$$D_{H/H_0}(z) = \det_{\mathcal{H}}\big((H - z\, I_{\mathcal{H}})(H_0 - z\, I_{\mathcal{H}})^{-1}\big) = \det_{\mathcal{H}}\big(I_{\mathcal{H}} + V(H_0 - z\, I_{\mathcal{H}})^{-1}\big).$$

Then

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

and

$$\int_{\mathbb{R}} |\xi(\lambda; H, H_0)|\, d\lambda \leqslant \|H - H_0\|_{\mathcal{B}_1(\mathcal{H})},$$

$$\int_{\mathbb{R}} \xi(\lambda; H, H_0)\, d\lambda = \operatorname{tr}_{\mathcal{H}}(H - H_0).$$

A Short Course on the SSF ξ (contd.):

Note. Formula $(*)$ remains **valid** in the **relative trace class case**, where $V(H_0 - zI_{\mathcal{H}})^{-1} \in \mathcal{B}_1(\mathcal{H})$. But in this case one only has

$$\int_{\mathbb{R}} \frac{|\xi(\lambda; H, H_0)|\, d\lambda}{1+\lambda^2} < \infty$$

(and no longer $\xi(\,\cdot\,; H, H_0) \in L^1(\mathbb{R}; d\lambda)$).

Similar, but slightly more involved formulas also work in the most general case where H and H_0 are only **resolvent comparable,** i.e.,

$$\big[(H - z\, I_{\mathcal{H}})^{-1} - (H_0 - z\, I_{\mathcal{H}})^{-1}\big] \in \mathcal{B}_1(\mathcal{H}).$$

Note. The physicist **Ilya Lifshitz** introduced $\xi(\,\cdot\,; H, H_0)$ first for **rank-one** perturbations V. **Mark Krein** then treated the **trace class** case, $V \in \mathcal{B}_1(\mathcal{H})$, **"one rank at a time"**.

A Short Course on the SSF ξ (contd.):

If $\dim(\operatorname{ran}(E_{H_0}(a-\epsilon, b+\epsilon))) < \infty$, then

$$\xi(b-0; H, H_0) - \xi(a+0; H, H_0) = \dim(\operatorname{ran}(E_{H_0}(a,b))) - \dim(\operatorname{ran}(E_H(a,b))). \quad (**)$$

Note. Again, formula $(**)$ remains **valid** in the **relative trace class case**, where $V(H_0 - zI_{\mathcal{H}})^{-1} \in \mathcal{B}_1(\mathcal{H})$.

Away from $\sigma_{ess}(H_0) = \sigma_{ess}(H)$, $\xi(\lambda; H, H_0)$ is **piecewise constant:**

Counting multiplicity: Suppose $\lambda_0 \in \mathbb{R}\backslash\{\sigma_{ess}(H_0)\}$. Then,

$$\xi(\lambda_0 + 0; H, H_0) - \xi(\lambda_0 - 0; H, H_0) = m(H_0; \lambda_0) - m(H; \lambda_0),$$

where $m(T, \lambda) \in \mathbb{N} \cup \{0\}$ denotes the multiplicity of the eigenvalue $\lambda \in \mathbb{R}$ of $T = T^*$.

Thus, for energies λ away from $\sigma_{ess}(H_0)$, $\xi(\lambda; H, H_0)$ represents the **difference** of two **eigenvalue counting functions.**

A Short Course on the SSF ξ (contd.):

The spectral shift function is only determined up to a **constant**.

Assuming H_0, H to be bounded from below

$$H_0 \geq cI_{\mathcal{H}},$$

the standard way to fix the **constant** is to impose the **normalization**

$$\xi(\lambda; H, H_0) = 0, \quad \lambda < \inf(\sigma(H_0) \cup \sigma(H)).$$

Moreover, in the semibounded case, one has the "chain rule",

$$\xi(\lambda; H_2, H_0) = \xi(\lambda; H_2, H_1) + \xi(\lambda; H_1, H_0).$$

A Short Course on the SSF ξ (contd.):

Scattering theory: The Birman–Krein formula

Let $S(H, H_0)$ be the scattering operator for the pair (H, H_0). Then

$$S(H, H_0) = \int_{\sigma_{ac}(H_0)}^{\oplus} S(\lambda; H, H_0)\, d\lambda,$$

where $S(\lambda; H, H_0)$ is the fixed energy scattering operator (sweeping spectral multiplicity issues of H_0 under the rug!). Then the **Birman–Krein formula** holds,

$$\xi(\lambda; H, H_0) = -\frac{1}{2\pi i} \ln(\det(S(\lambda; H, H_0)) \text{ for a.e. } \lambda \in \sigma_{ac}(H_0).$$

Example. If $H_0 = -(d^2/dx^2)$, $H = -(d^2/dx^2) + V(\cdot)$ in $L^2([0,\infty); dx)$, $V \in L^1([0,\infty); (1+|x|)dx)$, real-valued, then

$$D_{H/H_0}(z) = \text{the half-line } \textbf{Jost} \text{ function},$$

and

$$\xi(\lambda; H, H_0) \text{ equals the } \textbf{scattering phase shift function} \text{ for a.e. } \lambda \in \sigma_{ac}(H_0).$$

Connections Between ξ, Traces, and Determinants

Suppose H_0 and H are self-adjoint in $\mathcal{H}$ and satisfy

$$\big[(H - z\, I_{\mathcal{H}})^{-1} - (H_0 - z\, I_{\mathcal{H}})^{-1}\big] \in \mathcal{B}_1(\mathcal{H}) \text{ for some (hence, all) } z \in \rho(H_0) \cap \rho(H).$$

Since V " $=$ " $H - H_0$ is self-adjoint, we can always factor it as $V = AB = BA$ (e.g., using the spectral theorem), assuming

$$B(H_0 - z\, I_{\mathcal{H}})^{-1}, \ \overline{(H_0 - z\, I_{\mathcal{H}})^{-1} A} \in \mathcal{B}_2(\mathcal{H}), \quad z \in \mathbb{C}\backslash\mathbb{R},$$

and either:

(i) $\overline{B(H_0 - z\, I_{\mathcal{H}})^{-1} A} \in \mathcal{B}_1(\mathcal{H})$, $z \in \mathbb{C}\backslash\mathbb{R}$, or

(ii) $\overline{B(H_0 - z\, I_{\mathcal{H}})^{-1} A} \in \mathcal{B}_2(\mathcal{H})$, $z \in \mathbb{C}\backslash\mathbb{R}$.

One can then define **perturbation determinants** for $z \in \mathbb{C}\backslash\mathbb{R}$,

(i) $D_{H/H_0}(z) = \det_{\mathcal{H}}\big(I_{\mathcal{H}} + \overline{B(H_0 - z\, I_{\mathcal{H}})^{-1} A}\big)$ (Fredholm det.),

(ii) $D_{2,H/H_0}(z) = \det_{2,\mathcal{H}}\big(I_{\mathcal{H}} + \overline{B(H_0 - z\, I_{\mathcal{H}})^{-1} A}\big)$ (modified Fredholm det.).

Connections Between ξ, Traces, and Dets. (contd.)

In these cases,

$$\begin{aligned} -\frac{d}{dz}\ln(D_{H/H_0}(z)) &= \operatorname{tr}_{\mathcal{H}}\big((H - zI_{\mathcal{H}})^{-1} - (H_0 - zI_{\mathcal{H}})^{-1}\big) \\ &= -\int_{\mathbb{R}} \frac{\xi(\lambda; H, H_0)}{(\lambda - z)^2}\, d\lambda, \end{aligned}$$

and

$$\begin{aligned} -\frac{d}{dz}\ln(D_{2,H/H_0}(z)) &= \operatorname{tr}_{\mathcal{H}}\big((H - zI_{\mathcal{H}})^{-1} - (H_0 - zI_{\mathcal{H}})^{-1} \\ &\quad + (H_0 - z\, I_{\mathcal{H}})^{-1} V (H_0 - z\, I_{\mathcal{H}})^{-1}\big) \\ &= -\int_{\mathbb{R}} \frac{\xi(\lambda; H, H_0)}{(\lambda - z)^2}\, d\lambda + \operatorname{tr}_{\mathcal{H}}\big((H_0 - z\, I_{\mathcal{H}})^{-1} V (H_0 - z\, I_{\mathcal{H}})^{-1}\big). \end{aligned}$$

Applications to 1d Schrödinger Operators

Consider the Laplacian H_0 and a quadratic form perturbation H of it in $L^2(\mathbb{R}; dx)$:

$$H_0 = -\Delta, \quad \operatorname{dom}(H_0) = H^2(\mathbb{R}), \quad H = -\Delta +_q V,$$

where $V \in L^1(\mathbb{R}; dx)$ is real-valued. Here $+_q$ abbreviates the **form sum**.
Next, we factor

$$V(x) = u(x)v(x), \text{ where } v(x) = |V(x)|^{1/2}, \; u(x) = v(x)\,\mathrm{sgn}[V(x)], \quad x \in \mathbb{R}.$$

Then (with $I := I_{L^2(\mathbb{R};dx)}$),

(i) $\overline{u(H_0 - z\,I)^{-1}v} \in \mathcal{B}_1(L^2(\mathbb{R}; dx)), \quad z \in \mathbb{C}\backslash[0, \infty)$.

(ii) H and H_0 have a **trace class resolvent difference**,

$$\big[(H - z\,I)^{-1} - (H_0 - z\,I)^{-1}\big] \in \mathcal{B}_1\big(L^2(\mathbb{R}; dx)\big), \quad z \in \mathbb{R}\backslash\sigma(H).$$

(iii) $(H_0 - z\,I)^{-1}V(H_0 - z\,I)^{-1} \in \mathcal{B}_1\big(L^2(\mathbb{R}; dx)\big), \quad z \in \mathbb{C}\backslash[0, \infty)$.

(iv) For $z \in \mathbb{C}\backslash\sigma(H)$,

$$\operatorname{tr}\big((H - z\,I)^{-1} - (H_0 - z\,I)^{-1}\big) = -\frac{d}{dz}\ln\big(\det\big(I + \overline{u(H_0 - z\,I)^{-1}v}\big)\big).$$

Applications to 2d and 3d Schrödinger Operators

Again, consider the Laplacian H_0 and a quadratic form perturbation H of it in $L^2(\mathbb{R}^n; d^n x)$, $n = 2, 3$:

$$H_0 = -\Delta, \quad \mathrm{dom}(H_0) = H^2(\mathbb{R}^n), \quad H = -\Delta +_q V, \quad n = 2, 3,$$

where V is real-valued and $V \in \mathcal{R}_{2,\delta}$ for some $\delta > 0$ and $n = 2$, and $V \in \mathcal{R}_3 \cap L^1(\mathbb{R}^3; d^3x)$ for $n = 3$ and

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

$$\mathcal{R}_3 = \bigg\{ V : \mathbb{R}^3 \to \mathbb{R}, \text{ measurable} \,\bigg|\, \int_{\mathbb{R}^6} d^3x \, d^3x' \, |V(x')||V(x)||x - x'|^{-2} < \infty \bigg\},$$

Rollnik potentials in $\mathbb{R}^3$.

Again, $+_q$ abbreviates the **form sum**.

Appls. to 2d and 3d Schrödinger Operators (contd.)

Again, we factor

$$V(x) = u(x)v(x), \quad v(x) = |V(x)|^{1/2},\ u(x) = v(x)\,\mathrm{sgn}[V(x)], \quad x \in \mathbb{R}^n,\ n = 2, 3.$$

Then (with $I := I_{L^2(\mathbb{R}^n; d^n x)}$, $n = 2, 3$),

(i) $\overline{u(H_0 - z\,I)^{-1} v} \in \mathcal{B}_2(L^2(\mathbb{R}^n; d^n x)), \quad z \in \mathbb{C}\backslash[0, \infty),\ n = 2, 3.$

(ii) H and H_0 have a **trace class resolvent difference**,

$$\big[(H - z\,I)^{-1} - (H_0 - z\,I)^{-1}\big] \in \mathcal{B}_1\big(L^2(\mathbb{R}^n; d^n x)\big), \quad z \in \mathbb{R}\backslash\sigma(H),\ n = 2, 3.$$

(iii) $(H_0 - z\,I)^{-1} V (H_0 - z\,I)^{-1} \in \mathcal{B}_1\big(L^2(\mathbb{R}^n; d^n x)\big), \quad z \in \mathbb{C}\backslash[0, \infty),\ n = 2, 3.$

(iv) For $z \in \mathbb{C}\backslash\sigma(H)$,

$$\begin{aligned} &\mathrm{tr}\,\big((H - z\,I)^{-1} - (H_0 - z\,I)^{-1} + (H_0 - z\,I)^{-1} V (H_0 - z\,I)^{-1}\big) \\ &\quad = -\frac{d}{dz} \ln\big(\mathrm{det}_2\big(I + \overline{u(H_0 - z\,I)^{-1} v}\big)\big). \end{aligned}$$

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Approximations in Trace Ideals and Continuity of Spectral Shift Functions: Motivation

In our attempt to study the Witten index for higher-dimensional massless Dirac-type operators, we needed various approximation results which were not available in the literature. More importantly, those results should prove useful in a variety of other situations.

The following is based on:
A. Carey, F.G., G. Levitina, R. Nichols, D. Potapov, and F. Sukochev, J. Spectral Theory **6**, 747–779 (2016).

Motivation (contd.)

To describe the first such result, assume that A, B, A_n, B_n, $n \in \mathbb{N}$, are self-adjoint operators in a complex, separable Hilbert space $\mathcal{H}$, and suppose that

$$\operatorname*{s-lim}_{n\to\infty}(A_n - z_0 I_{\mathcal{H}})^{-1} = (A - z_0 I_{\mathcal{H}})^{-1},$$
$$\operatorname*{s-lim}_{n\to\infty}(B_n - z_0 I_{\mathcal{H}})^{-1} = (B - z_0 I_{\mathcal{H}})^{-1}$$

for some $z_0 \in \mathbb{C}\backslash\mathbb{R}$. Fix $m \in \mathbb{N}$, m odd, $p \in [1,\infty)$, and assume that for all $a \in \mathbb{R}\backslash\{0\}$,

$$T(a,m) := \big[(A - aiI_{\mathcal{H}})^{-m} - (B - aiI_{\mathcal{H}})^{-m}\big] \in \mathcal{B}_p(\mathcal{H}),$$
$$T_n(a,m) := \big[(A_n - aiI_{\mathcal{H}})^{-m} - (B_n - aiI_{\mathcal{H}})^{-m}\big] \in \mathcal{B}_p(\mathcal{H}),$$
$$\lim_{n\to\infty} \| T_n(a,m) - T(a,m)\|_{\mathcal{B}_p(\mathcal{H})} = 0.$$

Then for any function f in the class $\mathfrak{F}_m(\mathbb{R}) \supset C_0^\infty(\mathbb{R})$ (details later),

$$\lim_{n\to\infty} \big\|[f(A_n) - f(B_n)] - [f(A) - f(B)]\big\|_{\mathcal{B}_p(\mathcal{H})} = 0.$$

Motivation (contd.)

Moreover, for each $f \in \mathfrak{F}_m(\mathbb{R})$, $p \in [1,\infty)$, we prove the existence of constants $a_1, a_2 \in \mathbb{R}\backslash\{0\}$ and $C = C(f, m, a_1, a_2) \in (0,\infty)$ such that

$$\|f(A) - f(B)\|_{\mathcal{B}_p(\mathcal{H})} \leq C\Big(\big\|(A - a_1 iI_{\mathcal{H}})^{-m} - (B - a_1 iI_{\mathcal{H}})^{-m}\big\|_{\mathcal{B}_p(\mathcal{H})} + \big\|(A - a_2 iI_{\mathcal{H}})^{-m} - (B - a_2 iI_{\mathcal{H}})^{-m}\big\|_{\mathcal{B}_p(\mathcal{H})}\Big),$$

which permits the use of differences of higher powers $m \in \mathbb{N}$ of resolvents to **control** the $\|\cdot\|_{\mathcal{B}_p(\mathcal{H})}$-norm of the left-hand side $[f(A) - f(B)]$ for $f \in \mathfrak{F}_m(\mathbb{R})$.

Here, the class of functions $\mathfrak{F}_m(\mathbb{R})$, $m \in \mathbb{N}$ (introduced by **Yafaev** '05), is given by

$$\mathfrak{F}_m(\mathbb{R}) := \Big\{f \in C^2(\mathbb{R}) \,\Big|\, f^{(\ell)} \in L^\infty(\mathbb{R});\ \text{there exists } \varepsilon > 0 \text{ and } f_0 = f_0(f) \in \mathbb{C} \text{ such that } \big(d^\ell/d\lambda^\ell\big)\big[f(\lambda) - f_0\lambda^{-m}\big] \underset{|\lambda|\to\infty}{=} O\big(|\lambda|^{-\ell-m-\varepsilon}\big),\ \ell = 0,1,2\Big\}.$$

(It is implied that $f_0 = f_0(f)$ is the same as $\lambda \to \pm\infty$.) One observes that

$$\mathfrak{F}_m(\mathbb{R}) \supset C_0^\infty(\mathbb{R}),\ m \in \mathbb{N},$$
$$f(\lambda) \underset{|\lambda|\to\infty}{=} f_0\lambda^{-m} + O\big(|\lambda|^{-m-\epsilon}\big), \qquad f \in \mathfrak{F}_m(\mathbb{R}).$$

Motivation (contd.)

Our second result concerns the continuity of spectral shift functions $\xi(\,\cdot\,; B, B_0)$ associated with a pair of self-adjoint operators (B, B_0) in $\mathcal{H}$ w.r.t. the operator parameter B. Assume that A_0 and B_0 are fixed self-adjoint operators in $\mathcal{H}$, and there exists $m \in \mathbb{N}$, $m \in \mathbb{N}$ odd, such that, $\big[(B_0 - zI_{\mathcal{H}})^{-m} - (A_0 - zI_{\mathcal{H}})^{-m}\big] \in \mathcal{B}_1\big(\mathcal{H}\big)$, $z \in \mathbb{C}\backslash\mathbb{R}$. For T self-adjoint in $\mathcal{H}$ we denote by $\Gamma_m(T)$ the set of all self-adjoint operators S in $\mathcal{H}$ for which the containment, $\big[(S - zI_{\mathcal{H}})^{-m} - (T - zI_{\mathcal{H}})^{-m}\big] \in \mathcal{B}_1(\mathcal{H})$, $z \in \mathbb{C}\backslash\mathbb{R}$, ($m \in \mathbb{N}$ odd is fixed), holds.

Suppose that $B_1 \in \Gamma_m(B_0)$ and let $\{B_\tau\}_{\tau\in[0,1]} \subset \Gamma_m(B_0)$ denote a continuous path (in a suitable topology on $\Gamma_m(B_0)$, details later) from B_0 to B_1 in $\Gamma_m(B_0)$. If $f \in L^\infty(\mathbb{R})$, then

$$\lim_{\tau\to 0^+} \|\xi(\,\cdot\,; B_\tau, A_0)f - \xi(\,\cdot\,; B_0, A_0)f\|_{L^1(\mathbb{R};(|\nu|^{m+1}+1)^{-1}d\nu)} = 0.$$

The fact that higher powers $m \in \mathbb{N}$, $m \geq 2$, of resolvents are involved, permits applications of this circle of ideas to elliptic partial differential operators in $\mathbb{R}^n$, $n \in \mathbb{N}$. The proofs of these results rest on double operator integral (DOI) techniques.

No spectral gaps are assumed to exist in B_0, B.

A 5 min. Course on Double Operator Integrals (DOI):

A brief timeout on DOIs:

Daletskij and S. G. Krein (1960'), Birman and Solomyak (1960–70'), Peller, dePagter, Sukochev (1990–05), and others.

Our main goals: (i) Given self-adjoint operators A and B and a Borel function f, represent $f(A) - f(B)$ as a **double Stieltjes integral** with respect to the spectral measures $dE_A(\lambda)$ and $dE_B(\mu)$.

(ii) Construct a **bounded transformer** to the effect, for a bounded Borel function $\phi(\lambda, \mu)$ we would like to define $\mathcal{J}_\phi^{A,B} : \mathcal{B}_1(\mathcal{H}) \to \mathcal{B}_1(\mathcal{H})$ so that

$$\mathcal{J}_\phi^{A,B}(T) = \int_{\mathbb{R}} \int_{\mathbb{R}} \phi(\lambda, \mu)\, dE_A(\lambda)\, T\, dE_B(\mu), \quad T \in \mathcal{B}_1(\mathcal{H}) \text{ (or } \mathcal{B}(\mathcal{H})).$$

A 5 min. Course on DOI (contd.):

If A, B are **self-adjoint** matrices in $\mathbb{C}^n$, then $A = \sum_{j=1}^n \lambda_j E_A(\{\lambda_j\})$ and $B = \sum_{k=1}^n \mu_k E_B(\{\mu_k\})$ imply:

$$f(A) - f(B) = \sum_{j=1}^n \sum_{k=1}^n [f(\lambda_j) - f(\mu_k)] E_A(\{\lambda_j\}) E_B(\{\mu_k\})$$

$$= \sum_{j=1}^n \sum_{k=1}^n \frac{f(\lambda_j) - f(\mu_k)}{\lambda_j - \mu_k} E_A(\{\lambda_j\})(\lambda_j - \mu_k) E_B(\{\mu_k\})$$

$$= \sum_{j=1}^n \sum_{k=1}^n \frac{f(\lambda_j) - f(\mu_k)}{\lambda_j - \mu_k}$$

$$\times E_A(\{\lambda_j\}) \left(\sum_{j'=1}^n \lambda_{j'} E_A(\{\lambda_{j'}\}) - \sum_{k'=1}^n \mu_{k'} E_B(\{\mu_{k'}\}) \right) E_B(\{\mu_k\})$$

$$= \sum_{j=1}^n \sum_{k=1}^n \frac{f(\lambda_j) - f(\mu_k)}{\lambda_j - \mu_k} E_A(\{\lambda_j\})(A - B) E_B(\{\mu_k\}).$$

A 5 min. Course on DOI (contd.):

The **Birman–Solomyak formula**:

$$f(A) - f(B) = \int_{\mathbb{R}} \int_{\mathbb{R}} \frac{f(\lambda) - f(\mu)}{\lambda - \mu} \, dE_A(\lambda) \, (A - B) \, dE_B(\mu).$$

More generally: For a bounded Borel function $\phi(\lambda, \mu)$ we would like to define a **bounded transformer** $\mathcal{J}_\phi^{A,B} : \mathcal{B}_1(\mathcal{H}) \to \mathcal{B}_1(\mathcal{H})$ so that

$$\mathcal{J}_\phi^{A,B}(T) = \int_{\mathbb{R}} \int_{\mathbb{R}} \phi(\lambda, \mu) \, dE_A(\lambda) \, T \, dE_B(\mu), \quad T \in \mathcal{B}_1(\mathcal{H}).$$

$$\mathcal{J}_\phi^{A,B}(T) = \int_{\mathbb{R}} \alpha(\lambda) \, dE_A(\lambda) \, T \int_{\mathbb{R}} \beta(\mu) \, dE_B(\mu) \ \text{ for } \ \phi(\lambda, \mu) = \alpha(\lambda) \, \beta(\mu),$$

$$\mathcal{J}_\phi^{A,B}(T) = \int_{\mathbb{R}} \alpha_s(A) \, T \, \beta_s(B) \, \nu(s) ds \ \text{ for } \ \boxed{\phi(\lambda, \mu) = \int_{\mathbb{R}} \alpha_s(\lambda) \, \beta_s(\mu) \, \nu(s) \, ds,}$$

where α_s, β_s are bounded Borel functions, $\int_{\mathbb{R}} \|\alpha_s\|_\infty \, \|\beta_s\|_\infty \, \nu(s) \, ds < \infty$.

The (**Wiener**) class of such ϕ's is denoted by $\mathfrak{A}_0$.

Approximations in Trace Ideals:

Denote by $\mathcal{J}_\phi^{A,B}$ the linear mapping defined by the double operator integral

$$\mathcal{J}_\phi^{A,B}(T) = \int_{\mathbb{R}}\int_{\mathbb{R}} \phi(\lambda,\mu)\, dE_A(\lambda)\, T\, dE_B(\mu), \quad T \in \mathcal{B}(\mathcal{H}),$$

where E_A, E_B are spectral measures corresponding to the self-adjoint operators A, B.
If $\phi(\lambda,\mu) = a_1(\lambda)a_2(\mu)$, $(\lambda,\mu) \in \mathbb{R}^2$, for some bounded functions a_1 and a_2 on $\mathbb{R}$, then

$$\mathcal{J}_\phi^{A,B}(T) = a_1(A)\,T\,a_2(B).$$

Depending on ϕ, the operator $\mathcal{J}_\phi^{A,B}(T)$ can be bounded. Below we describe a class of functions ϕ such that

$$\mathcal{J}_\phi^{A,B} : \mathcal{B}_p(\mathcal{H}) \to \mathcal{B}_p(\mathcal{H}),\ p \in [1,\infty), \quad \mathcal{J}_\phi^{A,B} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}),$$

is a bounded operator. We introduce

$$\mathfrak{M}_p := \big\{\phi \in L^\infty(\mathbb{R}^2; d\rho)\,\big|\, \mathcal{J}_\phi^{A,B} \in \mathcal{B}(\mathcal{B}_p(\mathcal{H}))\big\}, \quad p \in [1,\infty),$$
$$\mathfrak{M}_\infty := \big\{\phi \in L^\infty(\mathbb{R}^2; d\rho)\,\big|\, \mathcal{J}_\phi^{A,B} \in \mathcal{B}(\mathcal{B}(\mathcal{H}))\big\},$$

where $\rho = \rho_A \otimes \rho_B$ denotes the product measure of ρ_A and ρ_B, the latter are suitable (scalar-valued) control measures for E_A and E_B, respectively.

Approximations in Trace Ideals (contd.):

E.g., $\rho_A(\cdot) = \sum_{j\in J}(e_j, E_A(\cdot)e_j)_{\mathcal{H}}$, with $\{e_j\}_{j\in J}$ a complete orthonormal system in $\mathcal{H}$, $J \subseteq \mathbb{N}$ an appropriate index set, and analogously for ρ_B. In addition, we set

$$\|\phi\|_{\mathfrak{M}_p} := \big\|\mathcal{J}_\phi^{A,B}\big\|_{\mathcal{B}(\mathcal{B}_p(\mathcal{H}))},\ p\in[1,\infty), \quad \|\phi\|_{\mathfrak{M}_\infty} := \big\|\mathcal{J}_\phi^{A,B}\big\|_{\mathcal{B}(\mathcal{B}(\mathcal{H}))}.$$

We denote $\mathfrak{M} := \mathfrak{M}_1 = \mathfrak{M}_\infty$, and $\|\phi\|_{\mathfrak{M}} := \|\phi\|_{\mathfrak{M}_1} = \|\phi\|_{\mathfrak{M}_\infty}$, $\phi \in \mathfrak{M}$.

Theorem (Birman–Solomyak ’03).

Assume that A and B are self-adjoint operators in $\mathcal{H}$. If the function $\phi(\,\cdot\,,\,\cdot\,)$ admits a representation of the form

$$\phi(\lambda,\mu) = \int_\Omega \alpha(\lambda,t)\beta(\mu,t)\,d\eta(t), \quad (\lambda,\mu)\in\mathbb{R}^2,$$

where $(\Omega, d\eta(t))$ is an auxiliary measure space and

$$C_\alpha^2 := \sup_{\lambda\in\mathbb{R}} \int_\Omega |\alpha(\lambda,t)|^2\,d\eta(t) < \infty, \quad C_\beta^2 := \sup_{\mu\in\mathbb{R}} \int_\Omega |\beta(\mu,t)|^2\,d\eta(t) < \infty,$$

then $\phi\in\mathfrak{M}$ and

$$\|\phi\|_{\mathfrak{M}} \leq C_\alpha C_\beta.$$

Approximations in Trace Ideals (contd.):

Theorem (Birman–Solomyak '03).

Assume that A and B are self-adjoint operators in $\mathcal{H}$. If there exist $0 \leq m_1 < 1$ and $1 < m_2$ such that

$$\sup_{\mu \in \mathbb{R}} \int_{\mathbb{R}} \big(|\xi|^{m_1} + |\xi|^{m_2}\big) \big|\widehat{\phi}(\xi, \mu)\big|^2 \, d\xi = C_0^2 < \infty,$$

where $\widehat{\phi}(\xi, \mu)$ stands for the partial Fourier transform of ϕ with respect to the first variable,

$$\widehat{\phi}(\xi, \mu) = (2\pi)^{-1} \int_{\mathbb{R}} \phi(\lambda, \mu) e^{-i\xi\lambda} \, d\lambda, \quad (\xi, \mu) \in \mathbb{R}^2,$$

then $\phi \in \mathfrak{M}$ and

$$\|\phi\|_{\mathfrak{M}} \leq C C_0,$$

where the constant $C = C(m_1, m_2) > 0$ does not depend on E_A or E_B.

Approximations in Trace Ideals (contd.):

Theorem (Ya '05).

Assume that A and B are self-adjoint operators in $\mathcal{H}$. Suppose that the function $K(\lambda, \mu)$ on $\mathbb{R}^2$ satisfies

$$|K(\lambda, \mu)| \leq C_K < \infty, \quad (\lambda, \mu) \in \mathbb{R}^2,$$

and is differentiable with respect to λ with

$$\left| \frac{\partial K(\lambda, \mu)}{\partial \lambda} \right| \leq \widetilde{C}_K \big(1 + \lambda^2\big)^{-1}, \quad (\lambda, \mu) \in \mathbb{R}^2,$$

where the constant $\widetilde{C}_K$ is independent of μ. Assume, in addition, that for every fixed $\mu \in \mathbb{R}$

$$\lim_{\lambda \to -\infty} K(\lambda, \mu) = \lim_{\lambda \to +\infty} K(\lambda, \mu)$$

(the limits exist). Then $\mathcal{J}_K^{A,B} \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$ and $\mathcal{J}_K^{A,B} \in \mathcal{B}(\mathcal{B}_p(\mathcal{H}))$, $p \in [1, \infty)$.

Approximations in Trace Ideals (contd.):

Corollary.

The norms $\|\mathcal{J}_K^{A,B}\|_{\mathcal{B}(\mathcal{B}(\mathcal{H}))}$, $\|\mathcal{J}_K^{A,B}\|_{\mathcal{B}(\mathcal{B}_p(\mathcal{H}))}$, $p \in [1,\infty)$, do not depend on the spectral measures E_A and E_B.

To prove the norm bounds we now introduce the following assumption.

Hypothesis.

Assume that A and B are fixed self-adjoint operators in the Hilbert space $\mathcal{H}$, $p \in [1,\infty)$, and there exists $m \in \mathbb{N}$, m odd, such that for all $a \in \mathbb{R}\backslash\{0\}$,

$$\big[(B - aiI_{\mathcal{H}})^{-m} - (A - aiI_{\mathcal{H}})^{-m}\big] \in \mathcal{B}_p(\mathcal{H}) \text{ (resp., } \mathcal{B}(\mathcal{H})).$$

Given the results recalled thus far, **Yafaev '05** introduces a bijection $\varphi : \mathbb{R} \to \mathbb{R}$ satisfying for some $c > 0$ and $r > 0$,

$$\varphi \in C^2(\mathbb{R}), \quad \varphi(\lambda) = \lambda^m, \ |\lambda| \geq r, \quad \varphi'(\lambda) \geq c, \ \lambda \in \mathbb{R},$$

and then shows the following:

Approximations in Trace Ideals (contd.):

There exist $a_1, a_2 \in \mathbb{R}\backslash\{0\}$ and $C = C(a_1, a_2, m) \in (0, \infty)$ such that

$$\begin{aligned}
&\big\|(\varphi(A) - iI_{\mathcal{H}})^{-1} - (\varphi(B) - iI_{\mathcal{H}})^{-1}\big\|_{\mathcal{B}_p(\mathcal{H})} \\
&\quad \leq C\big(\big\|(A - a_1 iI_{\mathcal{H}})^{-m} - (B - a_1 iI_{\mathcal{H}})^{-m}\big\|_{\mathcal{B}_p(\mathcal{H})} \\
&\qquad + \big\|(A - a_2 iI_{\mathcal{H}})^{-m} - (B - a_2 iI_{\mathcal{H}})^{-m}\big\|_{\mathcal{B}_p(\mathcal{H})}\big),
\end{aligned}$$

and an analogous estimate for the uniform norm $\|\cdot\|_{\mathcal{B}(\mathcal{H})}$. Moreover, he proves

$$\begin{aligned}
&[f(A) - f(B)] \in \mathcal{B}_p(\mathcal{H}) \ \text{(resp., } [f(A) - f(B)] \in \mathcal{B}(\mathcal{H})\text{)}, \\
&\big\|f(A) - f(B)\|_{\mathcal{B}_p(\mathcal{H})} \leq C\big(\big\|(A - a_1 iI_{\mathcal{H}})^{-m} - (B - a_1 iI_{\mathcal{H}})^{-m}\big\|_{\mathcal{B}_p(\mathcal{H})} \\
&\quad + \big\|(A - a_2 iI_{\mathcal{H}})^{-m} - (B - a_2 iI_{\mathcal{H}})^{-m}\big\|_{\mathcal{B}_p(\mathcal{H})}\big), \quad f \in \mathfrak{F}_m(\mathbb{R}), \ p \in [1, \infty)
\end{aligned}$$

(and the corresponding estimate for the uniform norm $\|\cdot\|_{\mathcal{B}(\mathcal{H})}$). Here the constant $C = C(f, a_1, a_2, m) \in (0, \infty)$ is independent of $p \in [1, \infty)$. (This can be improved for $p \in (1, \infty)$.)

Approximations in Trace Ideals (contd.):

Let A_n, B_n, A, B be self-adjoint operators in the Hilbert space $\mathcal{H}$. Suppose $\phi(\,\cdot\,,\,\cdot\,)$ admits a representation of the form

$$\phi(\lambda,\mu) = \int_\Omega \alpha(\lambda,t)\beta(\mu,t)\,d\eta(t), \quad (\lambda,\mu)\in\mathbb{R}^2, \qquad (*)$$

where $(\Omega, d\eta(t))$ is an auxiliary measure space and

$$C_\alpha^2 := \sup_{\lambda\in\mathbb{R}} \int_\Omega |\alpha(\lambda,t)|^2\,d\eta(t) < \infty, \quad C_\beta^2 := \sup_{\mu\in\mathbb{R}} \int_\Omega |\beta(\mu,t)|^2\,d\eta(t) < \infty.$$

Set

$$a(t) := \int_{\mathbb{R}} \alpha(\lambda,t)\,dE_A(\lambda), \quad b(t) := \int_{\mathbb{R}} \beta(\mu,t)\,dE_B(\mu),$$

$$a_n(t) := \int_{\mathbb{R}} \alpha(\lambda,t)\,dE_{A_n}(\lambda), \quad b_n(t) := \int_{\mathbb{R}} \beta(\mu,t)\,dE_{B_n}(\mu), \quad n\in\mathbb{N},$$

Approximations in Trace Ideals (contd.):

and introduce

$$\varepsilon_n(v,\alpha) = \left[\int_\Omega \|a_n(t)v - a(t)v\|^2 \, d\eta(t) \right]^{1/2},$$
$$\delta_n(v,\beta) = \left[\int_\Omega \|b_n(t)v - b(t)v\|^2 \, d\eta(t) \right]^{1/2}, \quad n \in \mathbb{N}, \ v \in \mathcal{H},$$

and

$$\mathfrak{A}_r^s(E_A) := \{\phi \text{ as in } (*) \,|\, \lim_{n\to\infty} \varepsilon_n(v,\alpha) = 0, \ v \in \mathcal{H}\},$$
$$\mathfrak{A}_l^s(E_B) := \{\phi \text{ as in } (*) \,|\, \lim_{n\to\infty} \delta_n(v,\alpha) = 0, \ v \in \mathcal{H}\}.$$

We note that the definitions of the classes $\mathfrak{A}_r^s(E_A), \mathfrak{A}_l^s(E_A)$ impose certain restrictions on convergences $A_n \longrightarrow A$ and $B_n \longrightarrow B$ as well as on the properties of the function ϕ as in $(*)$.

Proposition.

If $\phi, \psi \in \mathfrak{A}_r^s(E_A)$ (respectively, $\phi, \psi \in \mathfrak{A}_l^s(E_B)$), then $(\phi + \psi) \in \mathfrak{A}_r^s(E_A)$ (respectively, $(\phi + \psi) \in \mathfrak{A}_l^s(E_B)$).

Approximations in Trace Ideals (contd.):

Proposition (Birman–Solomyak '73).

Let $\phi \in \mathfrak{A}_r^s(E_A) \cap \mathfrak{A}_l^s(E_B)$. Then for any $T \in \mathcal{B}_p(\mathcal{H})$, $p \in [1, \infty)$,

$$\lim_{n\to\infty} \big\| \mathcal{J}_\phi^{A_n,B_n}(T) - \mathcal{J}_\phi^{A,B}(T) \big\|_{\mathcal{B}_p(\mathcal{H})} = 0, \quad p \in [1, \infty).$$

Hypothesis.

Let A, B, A_n, B_n, $n \in \mathbb{N}$, be self-adjoint operators in a separable Hilbert space $\mathcal{H}$ and suppose that

$$\operatorname*{s-lim}_{n\to\infty} (A_n - z_0 I_{\mathcal{H}})^{-1} = (A - z_0 I_{\mathcal{H}})^{-1}, \quad \operatorname*{s-lim}_{n\to\infty} (B_n - z_0 I_{\mathcal{H}})^{-1} = (B - z_0 I_{\mathcal{H}})^{-1}, \quad (**)$$

for some $z_0 \in \mathbb{C} \backslash \mathbb{R}$.

Approximations in Trace Ideals (contd.):

Lemma.

Assume $(**)$. If there exist $0 \leq m_1 < 1$ and $1 < m_2$ such that

$$\sup_{\mu\in\mathbb{R}} \int_{\mathbb{R}} \left(|\xi|^{m_1} + |\xi|^{m_2}\right) \left|\widehat{\phi}(\xi,\mu)\right|^2 d\xi = C_0^2 < \infty,$$

where $\widehat{\phi}(\xi,\mu)$ stands for the partial Fourier transform of ϕ with respect to the first variable,

$$\widehat{\phi}(\xi,\mu) = (2\pi)^{-1} \int_{\mathbb{R}} \phi(\lambda,\mu) e^{-i\xi\lambda}\, d\lambda, \quad (\xi,\mu) \in \mathbb{R}^2,$$

then $\phi \in \mathfrak{A}_r^s(E_A)$.

Approximations in Trace Ideals (contd.):

Corollary.

Assume $(**)$. If a function K on $\mathbb{R}^2$ satisfies

$$|K(\lambda,\mu)| \leq C_K < \infty, \quad (\lambda,\mu) \in \mathbb{R}^2,$$

and is differentiable with respect to λ with

$$\left|\frac{\partial K(\lambda,\mu)}{\partial\lambda}\right| \leq \widetilde{C}_K \big(1+\lambda^2\big)^{-1}, \quad (\lambda,\mu) \in \mathbb{R}^2,$$

where the constant $\widetilde{C}_K$ is independent of μ. Assume, in addition, that for every fixed $\mu \in \mathbb{R}$

$$\lim_{\lambda\to-\infty} K(\lambda,\mu) = \lim_{\lambda\to+\infty} K(\lambda,\mu)$$

(the limits exist), then $K \in \mathfrak{A}_r^s(E_B)$.

Approximations in Trace Ideals (contd.):

Next, we strengthen the assumptions on the operators A_n, A, B_n, B, $n \in \mathbb{N}$:

Hypothesis.

In addition to $(**)$ we assume that for some $m \in \mathbb{N}$, m odd, $p \in [1, \infty)$, and every $a \in \mathbb{R}\backslash\{0\}$,

$$T(a) := \big[(A + iaI_{\mathcal{H}})^{-m} - (B + iaI_{\mathcal{H}})^{-m}\big] \in \mathcal{B}_p(\mathcal{H}),$$
$$T_n(a) := \big[(A_n + iaI_{\mathcal{H}})^{-m} - (B_n + iaI_{\mathcal{H}})^{-m}\big] \in \mathcal{B}_p(\mathcal{H}),$$

and

$$\lim_{n\to\infty} \|T_n(a) - T(a)\|_{\mathcal{B}_p(\mathcal{H})} = 0.$$

With this hypothesis in hand, the following theorem is the main result thus far:

Theorem.

Assume the above hypothesis. Then for any function $f \in \mathfrak{F}_m(\mathbb{R})$,

$$\lim_{n\to\infty} \big\|[f(A_n) - f(B_n)] - [f(A) - f(B)]\big\|_{\mathcal{B}_p(\mathcal{H})} = 0, \quad p \in [1, \infty).$$

Continuity of $\xi(\,\cdot\,; B, B_0)$ w.r.t. B:

Some remarks on powers of resolvents:

The case $m = 1$. If A and B are self-adjoint operators in $\mathcal{H}$ and for some $z_0 \in \mathbb{C}\backslash\mathbb{R}$,

$$[(A - z_0 I_{\mathcal{H}})^{-1} - (B - z_0 I_{\mathcal{H}})^{-1}] \in \mathcal{B}_1(\mathcal{H}),$$

then actually

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

a fact which follows from the well-known resolvent identity

$$\begin{aligned}(A - zI_{\mathcal{H}})^{-1} - (B - zI_{\mathcal{H}})^{-1} &= (A - z_0 I_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1} \\ &\quad \times \big[(A - z_0 I_{\mathcal{H}})^{-1} - (B - z_0 I_{\mathcal{H}})^{-1}\big](B - z_0 I_{\mathcal{H}})(B - zI_{\mathcal{H}})^{-1}, \\ &\qquad z, z_0 \in \rho(A) \cap \rho(B).\end{aligned}$$

However, an analogous result **cannot** hold for higher powers of the resolvent as the following remarkably simple example illustrates:

Continuity of $\xi(\,\cdot\,; B, B_0)$ w.r.t. B:

Example $m = 3$.

Suppose $\mathcal{H}$ is an infinite-dimensional Hilbert space, and let $P_j \in \mathcal{B}(\mathcal{H})$, $j \in \{1, 2\}$, be infinite-dimensional orthogonal projections with

$$P_1 P_2 = 0 \quad \text{and} \quad P_1 + P_2 = I_{\mathcal{H}}. \tag{6.1}$$

Set

$$A = \sqrt{3}(P_1 + P_2), \quad B = \sqrt{3}(P_1 - P_2). \tag{6.2}$$

Evidently, $A^2 = B^2 = 3I_{\mathcal{H}}$, and

$$(A - iI_{\mathcal{H}})^3 = A^3 - 3iA^2 + 3(-i)^2 A - i^3 I_{\mathcal{H}} = -8iI_{\mathcal{H}}. \tag{6.3}$$

Similarly, one obtains $(B - iI_{\mathcal{H}})^3 = -8iI_{\mathcal{H}}$, and consequently,

$$(A - iI_{\mathcal{H}})^{-3} - (B - iI_{\mathcal{H}})^{-3} = 0 \in \mathcal{B}_1(\mathcal{H}). \tag{6.4}$$

However, if $z \in \mathbb{C}\backslash\{i\}$, then

$$(A + zI_{\mathcal{H}})^3 = A^3 + 3zA^2 + 3z^2 A + z^3 I_{\mathcal{H}}. \tag{6.5}$$

Continuity of $\xi(\,\cdot\,; B, B_0)$ w.r.t. B:

Example $m = 3$ (contd.).

Taking, for example, $z = 3i$ in (6.5), one computes

$$(A + zI_{\mathcal{H}})^3 = A(A^2 + 3z^2 I_{\mathcal{H}}) + z(3A^2 + z^2 I_{\mathcal{H}}) = -24A, \tag{6.6}$$

and similarly,

$$(B + 3iI_{\mathcal{H}})^3 = -24B. \tag{6.7}$$

Computing inverses, one infers

$$(A + 3iI_{\mathcal{H}})^{-3} = -\frac{1}{24}A^{-1} = -\frac{1}{24\sqrt{3}}(P_1 + P_2), \tag{6.8}$$

$$(B + 3iI_{\mathcal{H}})^{-3} = -\frac{1}{24}B^{-1} = -\frac{1}{24\sqrt{3}}(P_1 - P_2), \tag{6.9}$$

so that

$$(A + 3iI_{\mathcal{H}})^{-3} - (B + 3iI_{\mathcal{H}})^{-3} = -\frac{1}{12\sqrt{3}}P_2 \notin \mathcal{B}_\infty(\mathcal{H}), \tag{6.10}$$

due to the fact that P_2 is an infinite-dimensional projection in $\mathcal{H}$.

Continuity of $\xi(\,\cdot\,; B, B_0)$ w.r.t. B:

Hypothesis.

Assume that A_0 and B_0 are fixed self-adjoint operators in the Hilbert space $\mathcal{H}$, and there exists $m \in \mathbb{N}$, m odd, such that,

$$\big[(B_0 - zI_{\mathcal{H}})^{-m} - (A_0 - zI_{\mathcal{H}})^{-m}\big] \in \mathcal{B}_1\big(\mathcal{H}\big), \quad z \in \mathbb{C}\backslash\mathbb{R}.$$

Note. One really **needs all** $z \in \mathbb{C}\backslash\mathbb{R}$ for $m \geq 2$.

We denote by $\varphi : \mathbb{R} \to \mathbb{R}$ a bijection satisfying for some $c > 0$,

$$\varphi \in C^2(\mathbb{R}), \quad \varphi(\lambda) = \lambda^m, \ |\lambda| \geq 1, \quad \varphi'(\lambda) \geq c.$$

Then by **Yafaev '05** one has the fact

$$\big[(\varphi(B_0) - iI_{\mathcal{H}})^{-1} - (\varphi(A_0) - iI_{\mathcal{H}})^{-1}\big] \in \mathcal{B}_1(\mathcal{H}). \qquad (*)$$

Following **Yafaev '05**, one introduces the class of sSSFs for the pair (B_0, A_0) via

$$\xi(\nu; B_0, A_0) = \xi(\varphi(\nu); \varphi(B_0), \varphi(A_0)), \quad \nu \in \mathbb{R},$$

Continuity of $\xi(\,\cdot\,; B, B_0)$ w.r.t. B (contd.):

implying

$$\xi(\,\cdot\,; B_0, A_0) \in L^1\big(\mathbb{R}; (|\nu|^{m+1} + 1)^{-1} d\nu\big)$$

since upon introducing the new variable

$$\mu = \varphi(\nu) \in \mathbb{R}, \quad \nu \in \mathbb{R},$$

the inclusion $(*)$ yields

$$\xi(\,\cdot\,; \varphi(B_0), \varphi(A_0)) \in L^1\big(\mathbb{R}; (|\mu|^2 + 1)^{-1} d\mu\big).$$

The change of variables $\nu \to \mu$ yields for the corresponding trace formula,

$$\begin{aligned}
\operatorname{tr}(f(B_0) - f(A_0)) &= \operatorname{tr}\big((f \circ \varphi^{-1})(\varphi(B_0)) - (f \circ \varphi^{-1})(\varphi(A_0))\big) \\
&= \int_{\mathbb{R}} d\mu\, (f \circ \varphi^{-1})'(\mu)\, \xi(\mu; \varphi(B_0), \varphi(A_0)) \\
&= \int_{\mathbb{R}} d\nu\, f'(\nu)\, \xi(\nu; B_0, A_0), \quad f \in \mathfrak{F}_m(\mathbb{R}).
\end{aligned}$$

Continuity of $\xi(\,\cdot\,; B, B_0)$ w.r.t. B (contd.):

We need an appropriate topology but start with a transitivity property: if $B \in \Gamma_m(A)$ and $C \in \Gamma_m(B)$, then $C \in \Gamma_m(A)$, as well.

For each $m \in \mathbb{N}$, $\Gamma_m(T)$ can be equipped with the family $\mathcal{D} = \{d_{m,z}\}_{z\in\mathbb{C}\backslash\mathbb{R}}$ of **pseudometrics** defined by

$$d_{m,z}(S_1, S_2) = \big\|(S_2 - zI_{\mathcal{H}})^{-m} - (S_1 - zI_{\mathcal{H}})^{-m}\big\|_{\mathcal{B}_1(\mathcal{H})}, \quad S_1, S_2 \in \Gamma_m(T).$$

For each fixed $\varepsilon > 0$, $z \in \mathbb{C}\backslash\mathbb{R}$, and $S \in \Gamma_m(T)$, define

$$B(S; d_{m,z}, \varepsilon) = \{S' \in \Gamma_m(T) \,|\, d_{m,z}(S, S') < \varepsilon\},$$

to be the ε-ball centered at S with respect to the pseudometric $d_{m,z}$.

Definition.

$\mathcal{T}_m(\mathcal{D}, T)$ is the topology on $\Gamma_m(T)$ with the subbasis

$$\mathfrak{B}_m(\mathcal{D}, T) = \{B(S; d_{m,z}, \varepsilon) \,|\, S \in \Gamma_m(T),\ z \in \mathbb{C}\backslash\mathbb{R},\ \varepsilon > 0\}.$$

That is, $\mathcal{T}_m(\mathcal{D}, T)$ is the smallest topology on $\Gamma_m(T)$ which contains $\mathfrak{B}_m(\mathcal{D}, T)$.

Continuity of $\xi(\,\cdot\,; B, B_0)$ w.r.t. B (contd.):

To state the main results of this section, we introduce one more hypothesis:

Hypothesis.

(i) Let A_0, B_0, and B_1 denote self-adjoint operators in $\mathcal{H}$ with $B_0, B_1 \in \Gamma_m(A_0)$ for some odd $m \in \mathbb{N}$, and let $\{B_\tau\}_{\tau\in[0,1]} \subset \Gamma_m(B_0)$ (and hence in $\Gamma_m(A_0)$) be a path from B_0 to B_1 in $\Gamma_m(B_0)$ depending continuously on $\tau \in [0,1]$ with respect to the topology $\mathcal{T}_m(\mathcal{D}, T)$ introduced in the previous definition.
(ii) Assume that $\varphi : \mathbb{R} \to \mathbb{R}$ is a bijection satisfying for some $c > 0$ and $r > 0$,

$$\varphi \in C^2(\mathbb{R}), \quad \varphi(\lambda) = \lambda^m,\ |\lambda| \geq r, \quad \varphi'(\lambda) \geq c,\ \lambda \in \mathbb{R}.$$

Proposition.

Assume this hypothesis. Then $\varphi(B_0) \in \Gamma_1(\varphi(A_0))$, and

$$\{\varphi(B_\tau)\}_{\tau\in[0,1]} \subset \Gamma_1(\varphi(B_0))$$

is a path from $\varphi(B_0)$ to $\varphi(B_1)$ in $\Gamma_1(\varphi(B_0))$ depending continuously on $\tau \in [0,1]$ with respect to the metric $d_{1,i}(\,\cdot\,,\,\cdot\,)$.

Continuity of $\xi(\,\cdot\,; B, B_0)$ w.r.t. B (contd.):

The following theorem represents the principal result of this section:

Theorem.

Assume the above hypothesis and let $\xi_0(\,\cdot\,; \varphi(B_0), \varphi(A_0))$ be a spectral shift function for the pair $(\varphi(B_0), \varphi(A_0))$. Then for each $\tau \in [0,1]$, there is a unique spectral shift function $\xi(\,\cdot\,; \varphi(B_\tau), \varphi(A_0))$ for the pair $(\varphi(B_\tau), \varphi(A_0))$ depending continuously on $\tau \in [0,1]$ in the $L^1(\mathbb{R}; (\lambda^2+1)^{-1}d\lambda)$-norm such that

$$\xi(\,\cdot\,; \varphi(B_0), \varphi(A_0)) = \xi_0(\,\cdot\,; \varphi(B_0), \varphi(A_0)).$$

Consequently,

$$\xi(\,\cdot\,; B_\tau, A_0) := \xi(\varphi(\cdot); \varphi(B_\tau), \varphi(A_0)),$$

the corresponding spectral shift function for the pair (B_τ, A_0), depends continuously on $\tau \in [0,1]$ in the $L^1(\mathbb{R}; (|\nu|^{m+1}+1)^{-1}d\nu)$-norm and satisfies

$$\xi(\,\cdot\,; B_0, A_0) = \xi_0(\varphi(\cdot); \varphi(B_0), \varphi(A_0)).$$

Continuity of $\xi(\,\cdot\,; B, B_0)$ w.r.t. B (contd.):

Remark.

If $\{\tau_n\}_{n=1}^{\infty} \subset [0,1]$ and $\tau_n \to 0$ as $n \to \infty$, then the previous theorem implies

$$\lim_{n\to\infty} \|\xi(\,\cdot\,; B_{\tau_n}, A_0) - \xi(\,\cdot\,; B_0, A_0)\|_{L^1(\mathbb{R};(|\nu|^{m+1}+1)^{-1}d\nu)} = 0.$$

In particular, there exists a subsequence of $\{\xi(\,\cdot\,; B_{\tau_n}, A_0)\}_{n\in\mathbb{N}}$ which converges pointwise a.e. to $\xi(\,\cdot\,; B_0, A_0)$ as $n \to \infty$. $\diamond$

Continuity of $\xi(\,\cdot\,; B, B_0)$ w.r.t. B (contd.):

We conclude with an elementary consequence:

Corollary.

Under the hypotheses in the above theorem, if $f \in L^\infty(\mathbb{R})$, then

$$\lim_{\tau\to 0^+} \|\xi(\,\cdot\,; B_\tau, A_0)f - \xi(\,\cdot\,; B_0, A_0)f\|_{L^1(\mathbb{R};(|\nu|^{m+1}+1)^{-1}d\nu)} = 0,$$

in particular,

$$\lim_{\tau\to 0^+} \int_{\mathbb{R}} \xi(\nu; B_\tau, A_0)d\nu\, g(\nu) = \int_{\mathbb{R}} \xi(\nu; B_0, A_0)d\nu\, g(\nu)$$

for all $g \in L^\infty(\mathbb{R})$ such that $\operatorname{ess.sup}_{\nu\in\mathbb{R}} \big|(|\nu|^{m+1} + 1)g(\nu)\big| < \infty$.