

# Non-commutative analysis — modern advances

Fedor Sukochev

University of NSW, AUSTRALIA

Samara State University, Samara, June 24, 2013

# Noncommutative analysis

**Noncommutative analysis** is an analysis of functions whose arguments do not commute and whose values do not commute. We will discuss

- differentiation,
- Taylor-type approximation,
- applications to mathematical physics / perturbation theory.

Functions are defined on **operators** acting in a separable Hilbert space (can think of finite matrices). In the first part of the talk,  $H$  and  $V$  are **self-adjoint**.  $H$  is an initial operator and  $V$  its perturbation.

Given a Borel function  $f : \mathbb{R} \mapsto \mathbb{C}$  bounded on the spectrum on  $H$ , the operator function  $f(H)$  is defined via the **spectral theorem** (functional calculus).

# Spectral theorem

(diagonalisation of an operator)

- Finite-dimensional case:  $H = H^*$  is a finite matrix with eigenvalues  $\{\lambda_k\}_{k=1}^n$ . If  $P_k$  is a projection onto the eigenspace corresponding to  $\lambda_k$ , then

$$H = \sum_{k=1}^n \lambda_k \cdot P_k.$$

- Infinite-dimensional case:  $H = H^*$  is an operator. There is a unique spectral measure  $E$  such that

$$H = \int_{\mathbb{R}} \lambda dE(\lambda) = \int_{\text{spectrum}(H)} \lambda dE(\lambda).$$

For Borel  $f : \mathbb{R} \mapsto \mathbb{C}$  bounded on  $\sigma(H)$ , the function of  $H$  is defined by

$$f(H) := \int_{\mathbb{R}} f(\lambda) dE(\lambda).$$

If  $H$  describes interactions between the atoms of a pure crystal and  $H + V$  of a crystal with impurities, then the **change in the free energy of a crystal** equals (here,  $\text{tr}$  is the standard trace)

$$\text{tr}[f(H + V) - f(H)],$$

for a small defect  $V$  (mathematically, if the trace above is well defined). Lifshits was looking for efficient formulas to compute the change in the free energy.

# Non-commutative Lipschitz estimates

- In 1953 M. G. Krein proved that if  $H$  and  $V$  are self-adjoint and  $V \in \mathfrak{S}^1$ , then  $f(H+V) - f(H) \in \mathfrak{S}^1$  for every  $f \in C_c^\infty$ . Here,  $\mathfrak{S}^p$  is the Schatten-von Neumann class.
- M.G. Krein asked (in the case  $p = 1$ ):  
Let  $V \in \mathfrak{S}^p$ ,  $1 \leq p \leq \infty$  and if  $f \in C^1(\mathbb{R})$ . Is it true that

$$f(H+V) - f(H) \in \mathfrak{S}^p?$$

- A positive answer was relatively simply found for  $p = 2$ .
- Yu. Farforovskaya (and later others, e.g. Davies, Peller) showed that the answer is negative for  $p = 1$  and  $p = \infty$  in 1972 and 1967, respectively.

## Theorem

The answer is *positive* if  $1 < p < \infty$  ( D. Potapov & F.S., *Acta Math.* 2011).

# Non-commutative Lipschitz estimates

- In 1953 M. G. Krein proved that if  $H$  and  $V$  are self-adjoint and  $V \in \mathfrak{S}^1$ , then  $f(H+V) - f(H) \in \mathfrak{S}^1$  for every  $f \in C_c^\infty$ . Here,  $\mathfrak{S}^p$  is the Schatten-von Neumann class.
- M.G. Krein asked (in the case  $p = 1$ ):  
Let  $V \in \mathfrak{S}^p$ ,  $1 \leq p \leq \infty$  and if  $f \in C^1(\mathbb{R})$ . **Is it true that**

$$f(H+V) - f(H) \in \mathfrak{S}^p?$$

- A positive answer was relatively simply found for  $p = 2$ .
- Yu. Farforovskaya (and later others, e.g. Davies, Peller) showed that the answer is negative for  $p = 1$  and  $p = \infty$  in 1972 and 1967, respectively.

## Theorem

The answer is **positive** if  $1 < p < \infty$  ( D. Potapov & F.S., *Acta Math.* 2011).

# Non-commutative Lipschitz estimates

- In 1953 M. G. Krein proved that if  $H$  and  $V$  are self-adjoint and  $V \in \mathfrak{S}^1$ , then  $f(H+V) - f(H) \in \mathfrak{S}^1$  for every  $f \in C_c^\infty$ . Here,  $\mathfrak{S}^p$  is the Schatten-von Neumann class.
- M.G. Krein asked (in the case  $p = 1$ ):  
Let  $V \in \mathfrak{S}^p$ ,  $1 \leq p \leq \infty$  and if  $f \in C^1(\mathbb{R})$ . **Is it true that**

$$f(H+V) - f(H) \in \mathfrak{S}^p?$$

- A positive answer was relatively simply found for  $p = 2$ .
- Yu. Farforovskaya (and later others, e.g. Davies, Peller) showed that the answer is negative for  $p = 1$  and  $p = \infty$  in 1972 and 1967, respectively.

## Theorem

The answer is **positive** if  $1 < p < \infty$  ( D. Potapov & F.S., *Acta Math.* 2011).

# Non-commutative Lipschitz estimates

- In 1953 M. G. Krein proved that if  $H$  and  $V$  are self-adjoint and  $V \in \mathfrak{S}^1$ , then  $f(H+V) - f(H) \in \mathfrak{S}^1$  for every  $f \in C_c^\infty$ . Here,  $\mathfrak{S}^p$  is the Schatten-von Neumann class.
- M.G. Krein asked (in the case  $p = 1$ ):  
Let  $V \in \mathfrak{S}^p$ ,  $1 \leq p \leq \infty$  and if  $f \in C^1(\mathbb{R})$ . **Is it true that**

$$f(H+V) - f(H) \in \mathfrak{S}^p?$$

- A positive answer was relatively simply found for  $p = 2$ .
- Yu. Farforovskaya (and later others, e.g. Davies, Peller) showed that the answer is negative for  $p = 1$  and  $p = \infty$  in 1972 and 1967, respectively.

## Theorem

The answer is **positive** if  $1 < p < \infty$  ( D. Potapov & F.S., *Acta Math.* 2011).



# Non-commutative Lipschitz estimates

- In 1953 M. G. Krein proved that if  $H$  and  $V$  are self-adjoint and  $V \in \mathfrak{S}^1$ , then  $f(H+V) - f(H) \in \mathfrak{S}^1$  for every  $f \in C_c^\infty$ . Here,  $\mathfrak{S}^p$  is the Schatten-von Neumann class.
- M.G. Krein asked (in the case  $p = 1$ ):  
Let  $V \in \mathfrak{S}^p$ ,  $1 \leq p \leq \infty$  and if  $f \in C^1(\mathbb{R})$ . **Is it true that**

$$f(H+V) - f(H) \in \mathfrak{S}^p?$$

- A positive answer was relatively simply found for  $p = 2$ .
- Yu. Farforovskaya (and later others, e.g. Davies, Peller) showed that the answer is negative for  $p = 1$  and  $p = \infty$  in 1972 and 1967, respectively.

## Theorem

The answer is **positive** if  $1 < p < \infty$  ( D. Potapov & F.S., *Acta Math.* 2011).

# Perturbation argument, in its simplest form

Let  $A = \sum_j \lambda_j E_j$  and  $B = \sum_k \mu_k F_k$ . We argue as follows

$$f(B) - f(A) =$$

$$\sum_{j,k} F_k (f(B) - f(A)) E_j =$$

$$\sum_{j,k} F_k f(B) E_j - F_k f(A) E_j =$$

$$\sum_{j,k} f(\mu_k) F_k E_j - f(\lambda_j) F_k E_j =$$

$$\sum_{j,k} (f(\mu_k) - f(\lambda_j)) F_k E_j =$$

$$\sum_{j,k} \psi_{jk} (\mu_k - \lambda_j) F_k E_j =$$

$$\sum_{j,k} \psi_{jk} (\mu_k F_k E_j - F_k \lambda_j E_j) =$$

$$\sum_{j,k} \psi_{jk} (F_k B E_j - F_k A E_j) =$$

$$\sum_{j,k} \psi_{jk} F_k (A - B) E_j.$$

Thus, we obtained

$$f(B) - f(A) = T_{\psi_f}(A - B),$$

$$T_{\phi}(X) = \sum_{j,k} \phi(\lambda_j, \mu_k) F_k X E_j$$

$$\psi_f(x, y) = \frac{f(x) - f(y)}{x - y}$$

# Perturbation argument, in its simplest form

Let  $A = \sum_j \lambda_j E_j$  and  $B = \sum_k \mu_k F_k$ . We argue as follows

$$f(B) - f(A) =$$

$$\sum_{j,k} F_k (f(B) - f(A)) E_j =$$

$$\sum_{j,k} F_k f(B) E_j - F_k f(A) E_j =$$

$$\sum_{j,k} f(\mu_k) F_k E_j - f(\lambda_j) F_k E_j =$$

$$\sum_{j,k} (f(\mu_k) - f(\lambda_j)) F_k E_j =$$

$$\sum_{j,k} \psi_{jk} (\mu_k - \lambda_j) F_k E_j =$$

$$\sum_{j,k} \psi_{jk} (\mu_k F_k E_j - F_k \lambda_j E_j) =$$

$$\sum_{j,k} \psi_{jk} (F_k B E_j - F_k A E_j) =$$

$$\sum_{j,k} \psi_{jk} F_k (A - B) E_j.$$

Thus, we obtained

$$f(B) - f(A) = T_{\psi_f}(A - B),$$

$$T_{\phi}(X) = \sum_{j,k} \phi(\lambda_j, \mu_k) F_k X E_j$$

$$\psi_f(x, y) = \frac{f(x) - f(y)}{x - y}$$

# Perturbation argument, in its simplest form

Let  $A = \sum_j \lambda_j E_j$  and  $B = \sum_k \mu_k F_k$ . We argue as follows

$$f(B) - f(A) =$$

$$\sum_{j,k} F_k (f(B) - f(A)) E_j =$$

$$\sum_{j,k} F_k f(B) E_j - F_k f(A) E_j =$$

$$\sum_{j,k} f(\mu_k) F_k E_j - f(\lambda_j) F_k E_j =$$

$$\sum_{j,k} (f(\mu_k) - f(\lambda_j)) F_k E_j =$$

$$\sum_{j,k} \psi_{jk} (\mu_k - \lambda_j) F_k E_j =$$

$$\sum_{j,k} \psi_{jk} (\mu_k F_k E_j - F_k \lambda_j E_j) =$$

$$\sum_{j,k} \psi_{jk} (F_k B E_j - F_k A E_j) =$$

$$\sum_{j,k} \psi_{jk} F_k (A - B) E_j.$$

Thus, we obtained

$$f(B) - f(A) = T_{\psi_f}(A - B),$$

$$T_{\phi}(X) = \sum_{j,k} \phi(\lambda_j, \mu_k) F_k X E_j$$

$$\psi_f(x, y) = \frac{f(x) - f(y)}{x - y}$$

# Perturbation argument, in its simplest form

Let  $A = \sum_j \lambda_j E_j$  and  $B = \sum_k \mu_k F_k$ . We argue as follows

$$f(B) - f(A) =$$

$$\sum_{j,k} F_k (f(B) - f(A)) E_j =$$

$$\sum_{j,k} F_k f(B) E_j - F_k f(A) E_j =$$

$$\sum_{j,k} f(\mu_k) F_k E_j - f(\lambda_j) F_k E_j =$$

$$\sum_{j,k} (f(\mu_k) - f(\lambda_j)) F_k E_j =$$

$$\sum_{j,k} \psi_{jk} (\mu_k - \lambda_j) F_k E_j =$$

$$\sum_{j,k} \psi_{jk} (\mu_k F_k E_j - F_k \lambda_j E_j) =$$

$$\sum_{j,k} \psi_{jk} (F_k B E_j - F_k A E_j) =$$

$$\sum_{j,k} \psi_{jk} F_k (A - B) E_j.$$

Thus, we obtained

$$f(B) - f(A) = T_{\psi_f}(A - B),$$

$$T_{\phi}(X) = \sum_{j,k} \phi(\lambda_j, \mu_k) F_k X E_j$$

$$\psi_f(x, y) = \frac{f(x) - f(y)}{x - y}$$

# Perturbation argument, in its simplest form

Let  $A = \sum_j \lambda_j E_j$  and  $B = \sum_k \mu_k F_k$ . We argue as follows

$$f(B) - f(A) =$$

$$\sum_{j,k} F_k (f(B) - f(A)) E_j =$$

$$\sum_{j,k} F_k f(B) E_j - F_k f(A) E_j =$$

$$\sum_{j,k} f(\mu_k) F_k E_j - f(\lambda_j) F_k E_j =$$

$$\sum_{j,k} (f(\mu_k) - f(\lambda_j)) F_k E_j =$$

$$\sum_{j,k} \psi_{jk} (\mu_k - \lambda_j) F_k E_j =$$

$$\sum_{j,k} \psi_{jk} (\mu_k F_k E_j - F_k \lambda_j E_j) =$$

$$\sum_{j,k} \psi_{jk} (F_k B E_j - F_k A E_j) =$$

$$\sum_{j,k} \psi_{jk} F_k (A - B) E_j.$$

Thus, we obtained

$$f(B) - f(A) = T_{\psi_f}(A - B),$$

$$T_{\phi}(X) = \sum_{j,k} \phi(\lambda_j, \mu_k) F_k X E_j$$

$$\psi_f(x, y) = \frac{f(x) - f(y)}{x - y}$$

# Perturbation argument, in its simplest form

Let  $A = \sum_j \lambda_j E_j$  and  $B = \sum_k \mu_k F_k$ . We argue as follows

$$f(B) - f(A) =$$

$$\sum_{j,k} F_k (f(B) - f(A)) E_j =$$

$$\sum_{j,k} F_k f(B) E_j - F_k f(A) E_j =$$

$$\sum_{j,k} f(\mu_k) F_k E_j - f(\lambda_j) F_k E_j =$$

$$\sum_{j,k} (f(\mu_k) - f(\lambda_j)) F_k E_j =$$

$$\sum_{j,k} \psi_{jk} (\mu_k - \lambda_j) F_k E_j =$$

$$\sum_{j,k} \psi_{jk} (\mu_k F_k E_j - F_k \lambda_j E_j) =$$

$$\sum_{j,k} \psi_{jk} (F_k B E_j - F_k A E_j) =$$

$$\sum_{j,k} \psi_{jk} F_k (A - B) E_j.$$

Thus, we obtained

$$f(B) - f(A) = T_{\psi_f}(A - B),$$

$$T_{\phi}(X) = \sum_{j,k} \phi(\lambda_j, \mu_k) F_k X E_j$$

$$\psi_f(x, y) = \frac{f(x) - f(y)}{x - y}$$

# Schur multipliers and Fourier multipliers

As we have seen on the previous frame, the analysis of the difference

$$f(B) - f(A)$$

can be reduced to the question about the behavior of the **Schur multiplier**

$$T_{\psi_f}, \text{ where } \psi_f(x, y) = \frac{f(x) - f(y)}{x - y}$$

on the element  $A - B \in \mathfrak{S}^p$ ,  $1 \leq p < \infty$ . The study of various classes of Schur multipliers on Schatten-von Neumann classes  $\mathfrak{S}^p$  is one of the active areas of Noncommutative Analysis. This study is a noncommutative counterpart of the classical Fourier analysis. We shall exploit this connection for the case when  $1 < p \neq 2 < \infty$ .



# A $\mathfrak{G}^2$ estimate is simple

The following lemma is well known:

Lemma (non-commutative Parseval's identity)

If  $X \in \mathfrak{G}^2$ , then

$$\|X\|_2^2 = \sum_{j,k} \|F_k X E_j\|_2^2,$$

where  $\{E_j\}$  and  $\{F_k\}$  are families of orthogonal projections.

- This lemma ensures that  $T_{\psi_f}$  is bounded on  $\mathfrak{G}^2$  as long as

$$\psi_f \in L^\infty \iff f' \in L^\infty.$$

- This explains the simplicity of the argument behind the Lipschitz estimate for  $p = 2$ .

# A $\mathfrak{S}^2$ estimate is simple

The following lemma is well known:

Lemma (non-commutative Parseval's identity)

If  $X \in \mathfrak{S}^2$ , then

$$\|X\|_2^2 = \sum_{j,k} \|F_k X E_j\|_2^2,$$

where  $\{E_j\}$  and  $\{F_k\}$  are families of orthogonal projections.

- This lemma ensures that  $T_{\psi_f}$  is **bounded on  $\mathfrak{S}^2$**  as long as

$$\psi_f \in L^\infty \iff f' \in L^\infty.$$

- This explains the simplicity of the argument behind the Lipschitz estimate **for  $p = 2$** .

# A $\mathfrak{S}^2$ estimate is simple

The following lemma is well known:

Lemma (non-commutative Parseval's identity)

If  $X \in \mathfrak{S}^2$ , then

$$\|X\|_2^2 = \sum_{j,k} \|F_k X E_j\|_2^2,$$

where  $\{E_j\}$  and  $\{F_k\}$  are families of orthogonal projections.

- This lemma ensures that  $T_{\psi_f}$  is bounded on  $\mathfrak{S}^2$  as long as

$$\psi_f \in L^\infty \iff f' \in L^\infty.$$

- This explains the simplicity of the argument behind the Lipschitz estimate for  $p = 2$ .

# Vector-valued Harmonic analysis in UMD-spaces

- The new approach to  $\mathfrak{S}^p$  have become possible due to recent (and not so recent) developments in the vector-valued Harmonic analysis.
- The key concept in this area is the concept of UMD (unconditional martingale differences) spaces introduced by Pisier and developed by Burkholder.
- One of the key results is the vector-valued Marcinkiewicz multiplier theorem due to J. Bourgain

## Theorem

*If  $X$  is a UMD Banach space, then the Fourier multiplier defined by*

$$(\widehat{T_m(f)})(k) = m_k \hat{f}(k), \quad k \in \mathbb{Z}$$

*is bounded on vector-valued Bochner space  $L^p(\mathbb{T}, X)$  if  $m$  is a bounded sequence and  $m$  is of bounded variation over every dyadic interval  $2^d \leq |k| < 2^{d+1}$  uniformly for  $d \in \mathbb{N}$ .*

# The new approach to $\mathfrak{S}^p$ with $1 < p < \infty$ , $p \neq 2$

Unlike the simple case  $p = 2$ , the approach of D. Potapov & F.S. [Acta Math., 2011] is based on vector valued Marcinkiewicz multiplier theorem and the following ideas:

## Lemma

There is a *rapidly decreasing* function  $h$  such that, for every  $\|f'\|_\infty \leq 1$ ,

$$\psi_f(x, y) = \frac{f(x) - f(y)}{x - y} = \int_{\mathbb{R}} h(\sigma) |f(x) - f(y)|^{i\sigma} |x - y|^{-i\sigma} d\sigma.$$

- The operator  $R_\sigma = T_{w_\sigma}$ , where  $w_\sigma(x, y) = |x - y|^{i\sigma}$  is linked with the **Calderon-Zygmund** theory of **vector-valued** singular integral operators, in particular, with the **Marcinkiewicz multiplier** theorem.
- The representation above allows to write our Schur multiplier as follows

$$T_{\psi_f} = \int_{\mathbb{R}} h(\sigma) \tilde{R}_\sigma \cdot R_{-\sigma} d\sigma.$$

# The new approach to $\mathfrak{S}^p$ with $1 < p < \infty$ , $p \neq 2$

Unlike the simple case  $p = 2$ , the approach of D. Potapov & F.S. [Acta Math., 2011] is based on vector valued Marcinkiewicz multiplier theorem and the following ideas:

## Lemma

There is a **rapidly decreasing** function  $h$  such that, for every  $\|f'\|_\infty \leq 1$ ,

$$\psi_f(x, y) = \frac{f(x) - f(y)}{x - y} = \int_{\mathbb{R}} h(\sigma) |f(x) - f(y)|^{i\sigma} |x - y|^{-i\sigma} d\sigma.$$

- The operator  $R_\sigma = T_{w_\sigma}$ , where  $w_\sigma(x, y) = |x - y|^{i\sigma}$  is linked with the **Calderon-Zygmund** theory of **vector-valued** singular integral operators, in particular, with the **Marcinkiewicz multiplier** theorem.
- The representation above allows to write our Schur multiplier as follows

$$T_{\psi_f} = \int_{\mathbb{R}} h(\sigma) \tilde{R}_\sigma \cdot R_{-\sigma} d\sigma.$$

# The new approach to $\mathfrak{S}^p$ with $1 < p < \infty$ , $p \neq 2$

Unlike the simple case  $p = 2$ , the approach of D. Potapov & F.S. [Acta Math., 2011] is based on vector valued Marcinkiewicz multiplier theorem and the following ideas:

## Lemma

There is a **rapidly decreasing** function  $h$  such that, for every  $\|f'\|_\infty \leq 1$ ,

$$\psi_f(x, y) = \frac{f(x) - f(y)}{x - y} = \int_{\mathbb{R}} h(\sigma) |f(x) - f(y)|^{i\sigma} |x - y|^{-i\sigma} d\sigma.$$

- The operator  $R_\sigma = T_{w_\sigma}$ , where  $w_\sigma(x, y) = |x - y|^{i\sigma}$  is linked with the **Calderon-Zygmund** theory of **vector-valued** singular integral operators, in particular, with the **Marcinkiewicz multiplier** theorem.
- The representation above allows to write our Schur multiplier as follows

$$T_{\psi_f} = \int_{\mathbb{R}} h(\sigma) \tilde{R}_\sigma \cdot R_{-\sigma} d\sigma.$$

# The new approach to $\mathfrak{S}^p$ with $1 < p < \infty$ , $p \neq 2$

Unlike the simple case  $p = 2$ , the approach of D. Potapov & F.S. [Acta Math., 2011] is based on vector valued Marcinkiewicz multiplier theorem and the following ideas:

## Lemma

There is a **rapidly decreasing** function  $h$  such that, for every  $\|f'\|_\infty \leq 1$ ,

$$\psi_f(x, y) = \frac{f(x) - f(y)}{x - y} = \int_{\mathbb{R}} h(\sigma) |f(x) - f(y)|^{i\sigma} |x - y|^{-i\sigma} d\sigma.$$

- The operator  $R_\sigma = T_{w_\sigma}$ , where  $w_\sigma(x, y) = |x - y|^{i\sigma}$  is linked with the **Calderon-Zygmund** theory of **vector-valued** singular integral operators, in particular, with the **Marcinkiewicz multiplier** theorem.
- The representation above allows to write our Schur multiplier as follows

$$T_{\psi_f} = \int_{\mathbb{R}} h(\sigma) \tilde{R}_\sigma \cdot R_{-\sigma} d\sigma.$$



# The new approach to $\mathfrak{S}^p$ with $1 < p < \infty$ , $p \neq 2$

computing the total variation of the sequence  $\lambda = \{n^{is}\}_{n>0}$  over dyadic intervals via the fundamental theorem of the calculus, we have

$$|n^{is} - (n+1)^{is}| \leq \frac{|s|}{n}, \quad n \geq 1$$

and thus immediately

$$\sum_{2^k \leq n \leq 2^{k+1}} |n^{is} - (n+1)^{is}| \leq |s|, \quad k \geq 0.$$

Together with the vector valued Marcinkiewicz multiplier theorem and **Transference Method** (developed, in particular, by Berkson and Gillespie), we infer that  $\|R_{-\sigma}\|_{\mathfrak{S}^p \rightarrow \mathfrak{S}^p} \leq (1 + |s|)$ . A similar estimate also holds for  $\tilde{R}_\sigma$ . This allows us to conclude that  $\|T_{\psi_f}\|_{\mathfrak{S}^p \rightarrow \mathfrak{S}^p} < \infty$ . We are done.

# Spectral shift function of M.G. Krein

Answering Lifshits's question, computing

$$\mathrm{tr}(f(H + V) - f(H)),$$

M.G. Krein introduced an object known now as a **spectral shift function of Krein** (the function  $\xi$  below).

**Theorem (M.G. Krein, 1953)**

If  $H$  and  $V$  are self-adjoint and  $V \in \mathfrak{S}^1$ , then there is  $L^1$ -function  $\xi = \xi_{H,V}$  such that

$$\mathrm{tr}(f(H + V) - f(H)) = \int_{\mathbb{R}} f'(t) \xi(t) dt,$$

for every  $f \in C_c^\infty$ .

# Construction of the Krein's function in case of finite trace

Let  $H, V \geq 0$ , let  $\tau$  be finite trace and let  $n_H(t) := \tau(E_H(t, \infty))$ ,  $t \in \mathbb{R}$ . It follows from the functional calculus that  $f(H) = -\int_0^\infty f(s) dE_H(s, \infty)$ . Taking the trace and integrating by parts, we obtain

$$\begin{aligned}\tau(f(H)) &= -\int_0^\infty f(s) dn_H(s) \\ &= -f(s)n_H(s)\Big|_0^\infty + \int_0^\infty f'(s)n_H(s)ds = \int_0^\infty f'(s)n_H(s)ds.\end{aligned}$$

Thus, we arrive at

$$\tau(f(H+V) - f(H)) = \int_0^\infty f'(s)(n_{H+V} - n_H)(s)ds.$$

# Construction of the Krein's function in case of finite trace

Let  $H, V \geq 0$ , let  $\tau$  be finite trace and let  $n_H(t) := \tau(E_H(t, \infty))$ ,  $t \in \mathbb{R}$ . It follows from the functional calculus that  $f(H) = -\int_0^\infty f(s) dE_H(s, \infty)$ . Taking the trace and integrating by parts, we obtain

$$\begin{aligned}\tau(f(H)) &= -\int_0^\infty f(s) dn_H(s) \\ &= -f(s)n_H(s)\Big|_0^\infty + \int_0^\infty f'(s)n_H(s)ds = \int_0^\infty f'(s)n_H(s)ds.\end{aligned}$$

Thus, we arrive at

$$\tau(f(H+V) - f(H)) = \int_0^\infty f'(s)(n_{H+V} - n_H)(s)ds.$$

# Construction of the Krein's function in case of finite trace

Let  $H, V \geq 0$ , let  $\tau$  be finite trace and let  $n_H(t) := \tau(E_H(t, \infty))$ ,  $t \in \mathbb{R}$ . It follows from the functional calculus that  $f(H) = -\int_0^\infty f(s) dE_H(s, \infty)$ . Taking the trace and integrating by parts, we obtain

$$\begin{aligned}\tau(f(H)) &= -\int_0^\infty f(s) dn_H(s) \\ &= -f(s)n_H(s)\Big|_0^\infty + \int_0^\infty f'(s)n_H(s)ds = \int_0^\infty f'(s)n_H(s)ds.\end{aligned}$$

Thus, we arrive at

$$\tau(f(H+V) - f(H)) = \int_0^\infty f'(s)(n_{H+V} - n_H)(s)ds.$$

# Construction of the Krein's function in case of finite trace

Let  $H, V \geq 0$ , let  $\tau$  be finite trace and let  $n_H(t) := \tau(E_H(t, \infty))$ ,  $t \in \mathbb{R}$ . It follows from the functional calculus that  $f(H) = -\int_0^\infty f(s)dE_H(s, \infty)$ . Taking the trace and integrating by parts, we obtain

$$\begin{aligned}\tau(f(H)) &= -\int_0^\infty f(s)dn_H(s) \\ &= -f(s)n_H(s)\Big|_0^\infty + \int_0^\infty f'(s)n_H(s)ds = \int_0^\infty f'(s)n_H(s)ds.\end{aligned}$$

Thus, we arrive at

$$\tau(f(H+V) - f(H)) = \int_0^\infty f'(s)(n_{H+V} - n_H)(s)ds.$$

# Construction of the Krein's function in case of finite trace

Let  $H, V \geq 0$ , let  $\tau$  be finite trace and let  $n_H(t) := \tau(E_H(t, \infty))$ ,  $t \in \mathbb{R}$ . It follows from the functional calculus that  $f(H) = -\int_0^\infty f(s) dE_H(s, \infty)$ . Taking the trace and integrating by parts, we obtain

$$\begin{aligned}\tau(f(H)) &= -\int_0^\infty f(s) dn_H(s) \\ &= -f(s)n_H(s)\Big|_0^\infty + \int_0^\infty f'(s)n_H(s)ds = \int_0^\infty f'(s)n_H(s)ds.\end{aligned}$$

Thus, we arrive at

$$\tau(f(H+V) - f(H)) = \int_0^\infty f'(s)(n_{H+V} - n_H)(s)ds.$$

# Construction of the Krein's function in case of finite trace

Let  $H, V \geq 0$ , let  $\tau$  be finite trace and let  $n_H(t) := \tau(E_H(t, \infty))$ ,  $t \in \mathbb{R}$ . It follows from the functional calculus that  $f(H) = -\int_0^\infty f(s) dE_H(s, \infty)$ . Taking the trace and integrating by parts, we obtain

$$\begin{aligned}\tau(f(H)) &= -\int_0^\infty f(s) dn_H(s) \\ &= -f(s)n_H(s)\Big|_0^\infty + \int_0^\infty f'(s)n_H(s) ds = \int_0^\infty f'(s)n_H(s) ds.\end{aligned}$$

Thus, we arrive at

$$\tau(f(H+V) - f(H)) = \int_0^\infty f'(s)(n_{H+V} - n_H)(s) ds.$$



# Construction of the Krein's function in case of finite trace

Let  $H, V \geq 0$ , let  $\tau$  be finite trace and let  $n_H(t) := \tau(E_H(t, \infty))$ ,  $t \in \mathbb{R}$ . It follows from the functional calculus that  $f(H) = -\int_0^\infty f(s)dE_H(s, \infty)$ . Taking the trace and integrating by parts, we obtain

$$\begin{aligned}\tau(f(H)) &= -\int_0^\infty f(s)dn_H(s) \\ &= -f(s)n_H(s)\Big|_0^\infty + \int_0^\infty f'(s)n_H(s)ds = \int_0^\infty f'(s)n_H(s)ds.\end{aligned}$$

Thus, we arrive at

$$\tau(f(H+V) - f(H)) = \int_0^\infty f'(s)(n_{H+V} - n_H)(s)ds.$$

# Construction of the Krein's function in case of finite trace

Let  $H, V \geq 0$ , let  $\tau$  be finite trace and let  $n_H(t) := \tau(E_H(t, \infty))$ ,  $t \in \mathbb{R}$ . It follows from the functional calculus that  $f(H) = -\int_0^\infty f(s) dE_H(s, \infty)$ . Taking the trace and integrating by parts, we obtain

$$\begin{aligned}\tau(f(H)) &= -\int_0^\infty f(s) dn_H(s) \\ &= -f(s)n_H(s)\Big|_0^\infty + \int_0^\infty f'(s)n_H(s)ds = \int_0^\infty f'(s)n_H(s)ds.\end{aligned}$$

Thus, we arrive at

$$\tau(f(H+V) - f(H)) = \int_0^\infty f'(s)(n_{H+V} - n_H)(s)ds.$$

# Spectral shift function explained

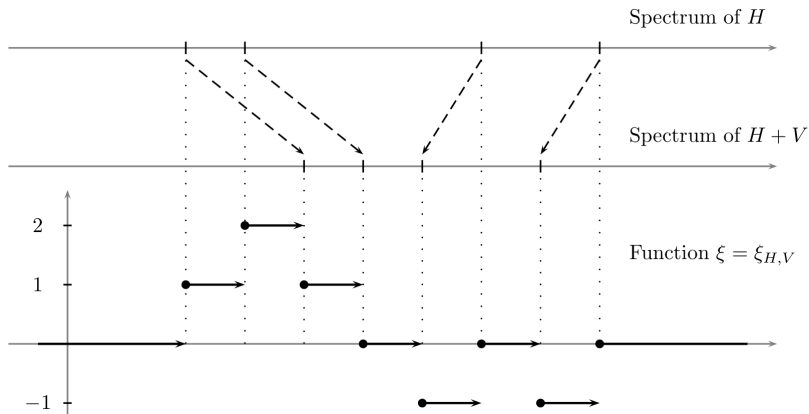


Figure: M.G. Krein spectral shift function explained

# L. Koplienko development of the trace formula

In 1984, L. Koplienko proved the following improvement of the M.G. Kreins trace formula:

## Theorem (Koplienko, 1984)

If  $H$  and  $V$  are self-adjoint and  $V \in \mathfrak{S}^2$ , then there is an  $L^1$ -function  $\eta$  (the spectral shift function of Koplienko) such that

$$\operatorname{tr}(R_2(f, H, V)) = \int_{\mathbb{R}} f''(t) \eta(t) dt, \quad \text{for every } f \in C_c^\infty,$$

$$\text{where } R_2(f, H, V) = f(H + V) - f(H) - \frac{d}{dt} [f(H_t)] \Big|_{t=0}.$$

- L. Koplienko also attempted to establish a version of the spectral shift formula for  $V \in \mathfrak{S}^p$  with  $p > 2$ .

# L. Koplienko development of the trace formula

In 1984, L. Koplienko proved the following improvement of the M.G. Kreins trace formula:

## Theorem (Koplienko, 1984)

If  $H$  and  $V$  are self-adjoint and  $V \in \mathfrak{S}^2$ , then there is an  $L^1$ -function  $\eta$  (the spectral shift function of Koplienko) such that

$$\operatorname{tr}(R_2(f, H, V)) = \int_{\mathbb{R}} f''(t) \eta(t) dt, \quad \text{for every } f \in C_c^\infty,$$

$$\text{where } R_2(f, H, V) = f(H + V) - f(H) - \frac{d}{dt} [f(H_t)] \Big|_{t=0}.$$

- L. Koplienko also attempted to establish a version of the spectral shift formula for  $V \in \mathfrak{S}^p$  with  $p > 2$ .

# L. Koplienko conjecture of 1984

The following result was **conjectured** by L. Koplienko in 1984

## Theorem

If  $H$  and  $V$  are self-adjoint and  $V \in \mathfrak{S}^n$ , then there is an  $L^1$ -function  $\eta_n = \eta_{n,H,V}$  such that

$$\operatorname{tr}(R_n(f, H, V)) = \int_{\mathbb{R}} f^{(n)}(t) \eta_n(t) dt, \quad \text{for every } f \in C_c^\infty,$$

$$\text{where } R_n(f, H, V) = f(H + V) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} [f(H_t)] \Big|_{t=0}.$$

- The conjecture is now **fully proved** by D. Potapov, A. Skripka & F. S., Invent. Math. (to appear).

# L. Koplienko conjecture of 1984

The following result was **conjectured** by L. Koplienko in 1984

## Theorem

If  $H$  and  $V$  are self-adjoint and  $V \in \mathfrak{S}^n$ , then there is an  $L^1$ -function  $\eta_n = \eta_{n,H,V}$  such that

$$\operatorname{tr}(R_n(f, H, V)) = \int_{\mathbb{R}} f^{(n)}(t) \eta_n(t) dt, \quad \text{for every } f \in C_c^\infty,$$

$$\text{where } R_n(f, H, V) = f(H + V) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} [f(H_t)] \Big|_{t=0}.$$

- The conjecture is now **fully proved** by D. Potapov, A. Skripka & F. S., Invent. Math. (to appear).

# Advanced estimates of higher order

- A complex combination of vector-valued harmonic analysis enabled the following result:

Theorem (D. Potapov, A. Skripka & F.S., Invent. Math. (to appear))

Let  $H$  and  $V$  be self-adjoint operators and let  $1 < p < \infty$ ,  $n > 1$ . *There is  $c_{n,p} > 0$  such that,*

- if  $V \in \mathfrak{S}^{np}$  then  $\left\| \frac{d^n}{dt^n} f(H + tV) \right\|_p \leq c_{n,p} \cdot \|V\|_{np}^n \cdot \|f^{(n)}\|_\infty$
- if  $V \in \mathfrak{S}^n$ , then  $\left| \operatorname{tr} \left( \frac{d^n}{dt^n} f(H + tV) \right) \right| \leq c_n \cdot \|V\|_n^n \cdot \|f^{(n)}\|_\infty$

- The result above lies at the core of our resolution of Kopljenko conjecture of 1984.



# Advanced estimates of higher order

- A complex combination of vector-valued harmonic analysis enabled the following result:

Theorem (D. Potapov, A. Skripka & F.S., Invent. Math. (to appear))

Let  $H$  and  $V$  be self-adjoint operators and let  $1 < p < \infty$ ,  $n > 1$ . *There is  $c_{n,p} > 0$  such that,*

- if  $V \in \mathfrak{S}^{np}$  then  $\left\| \frac{d^n}{dt^n} f(H + tV) \right\|_p \leq c_{n,p} \cdot \|V\|_{np}^n \cdot \|f^{(n)}\|_\infty$
- if  $V \in \mathfrak{S}^n$ , then  $\left| \operatorname{tr} \left( \frac{d^n}{dt^n} f(H + tV) \right) \right| \leq c_n \cdot \|V\|_n^n \cdot \|f^{(n)}\|_\infty$

- The result above lies at the core of our resolution of Koplienko conjecture of 1984.

# Advanced estimates of higher order

- A complex combination of vector-valued harmonic analysis enabled the following result:

Theorem (D. Potapov, A. Skripka & F.S., Invent. Math. (to appear))

Let  $H$  and  $V$  be self-adjoint operators and let  $1 < p < \infty$ ,  $n > 1$ . *There is  $c_{n,p} > 0$  such that,*

- if  $V \in \mathfrak{S}^{np}$  then  $\left\| \frac{d^n}{dt^n} f(H + tV) \right\|_p \leq c_{n,p} \cdot \|V\|_{np}^n \cdot \|f^{(n)}\|_\infty$
- if  $V \in \mathfrak{S}^n$ , then  $\left| \operatorname{tr} \left( \frac{d^n}{dt^n} f(H + tV) \right) \right| \leq c_n \cdot \|V\|_n^n \cdot \|f^{(n)}\|_\infty$

- The result above lies at the core of our resolution of Koplienko conjecture of 1984.

# Advanced estimates of higher order

- A complex combination of vector-valued harmonic analysis enabled the following result:

Theorem (D. Potapov, A. Skripka & F.S., Invent. Math. (to appear))

Let  $H$  and  $V$  be self-adjoint operators and let  $1 < p < \infty$ ,  $n > 1$ . *There is  $c_{n,p} > 0$  such that,*

- if  $V \in \mathfrak{S}^{np}$  then  $\left\| \frac{d^n}{dt^n} f(H + tV) \right\|_p \leq c_{n,p} \cdot \|V\|_{np}^n \cdot \|f^{(n)}\|_\infty$
- if  $V \in \mathfrak{S}^n$ , then  $\left| \operatorname{tr} \left( \frac{d^n}{dt^n} f(H + tV) \right) \right| \leq c_n \cdot \|V\|_n^n \cdot \|f^{(n)}\|_\infty$

- The result above lies **at the core of our resolution** of Koplienko conjecture of 1984.

# Koplienko spectral shift function for contractions

In 2008, F. Gesztesy, A. Pushnitski, and B. Simon conjectured that Koplienko result holds also for contractions. The conjecture was as follows (here and below  $H$  and  $V$  are not necessarily self-adjoint).

## Theorem

If  $H$  and  $V$  are such that  $H$  and  $H + V$  are *contractions* and  $V \in \mathfrak{G}^2$ , then there is an  $L^1$ -function  $\eta = \eta_{H,V}$  such that

$$\mathrm{tr}(R_2(f, H, V)) = \int_{\mathbb{T}} f''(z) \eta(z) dz,$$

for every *polynomial*  $f$ .

- The conjecture is now *settled positively* by D. Potapov and F. S. (Comm. Math. Phys 2012).

# Koplienko spectral shift function for contractions

In 2008, F. Gesztesy, A. Pushnitski, and B. Simon conjectured that Koplienko result holds also for contractions. The conjecture was as follows (here and below  $H$  and  $V$  are not necessarily self-adjoint).

## Theorem

If  $H$  and  $V$  are such that  $H$  and  $H + V$  are *contractions* and  $V \in \mathfrak{G}^2$ , then there is an  $L^1$ -function  $\eta = \eta_{H,V}$  such that

$$\mathrm{tr}(R_2(f, H, V)) = \int_{\mathbb{T}} f''(z) \eta(z) dz,$$

for every *polynomial*  $f$ .

- The conjecture is now *settled positively* by D. Potapov and F. S. (Comm. Math. Phys 2012).

# Higher order spectral shift for contractions

The following result shows the existence of spectral shift function for  $n \geq 3$  in case of contractions.

## Theorem

If  $H$  and  $V$  are such that  $H$  and  $H + V$  are *contractions* and  $V \in \mathfrak{S}^n$ ,  $n \geq 3$ , then there is a function  $\eta_n = \eta_{n,H,V} \in L^1(\mathbb{T})$  such that

$$\mathrm{tr}(R_n(f, H, V)) = \int_{\mathbb{T}} f^{(n)}(z) \eta_n(z) dz,$$

for every *polynomial*  $f$ .

- Theorem above is now *fully proved* by D. Potapov, A. Skripka & F. S., London Math. Soc. (to appear).

# Higher order spectral shift for contractions

The following result shows the existence of spectral shift function for  $n \geq 3$  in case of contractions.

## Theorem

If  $H$  and  $V$  are such that  $H$  and  $H + V$  are *contractions* and  $V \in \mathfrak{S}^n$ ,  $n \geq 3$ , then there is a function  $\eta_n = \eta_{n,H,V} \in L^1(\mathbb{T})$  such that

$$\mathrm{tr}(R_n(f, H, V)) = \int_{\mathbb{T}} f^{(n)}(z) \eta_n(z) dz,$$

for every *polynomial*  $f$ .

- Theorem above is now *fully proved* by D. Potapov, A. Skripka & F. S., London Math. Soc. (to appear).

# Advanced estimates of higher order in case of contractions

- The following results lies **at the core of the proof** of Theorem above.

Theorem (D. Potapov, A. Skripka & F.S., London Math. Soc. (to appear))

Let  $H$  and  $V$  be such that  $H$  and  $H + V$  are **contractions** and let  $n > 1$  and  $\alpha > n$ . **There is  $c_n > 0$**  such that for any polynomial  $f$ , the following estimates hold:

- if  $V \in \mathfrak{S}^\alpha$ , then  $\sup_{t_0 \in [0,1]} \left\| \frac{d^n}{dt^n} f(H + tV) \Big|_{t=t_0} \right\|_{\frac{\alpha}{n}} \leq c_n \|V\|_\alpha^n \|f^{(n)}\|_{L_\infty(\mathbb{T})}$  ;
- if  $V \in \mathfrak{S}^n$ , then  $\sup_{t_0 \in [0,1]} \left| \operatorname{tr} \left( \frac{d^n}{dt^n} f(H + tV) \Big|_{t=t_0} \right) \right| \leq c_n \cdot \|V\|_n^n \cdot \|f^{(n)}\|_{L_\infty(\mathbb{T})}$ .

- The two cases above are the ones of self-adjoints and unitaries, while the case of contractions reduces to the case of unitaries by applying the **Sz.-Nagy-Foiaş dilation theory**.
- However, the proofs can not be carried over from the self-adjoint case and **require an independent treatment** for the case of unitaries.



# Advanced estimates of higher order in case of contractions

- The following results lies **at the core of the proof** of Theorem above.

Theorem (D. Potapov, A. Skripka & F.S., London Math. Soc. (to appear))

Let  $H$  and  $V$  be such that  $H$  and  $H + V$  are **contractions** and let  $n > 1$  and  $\alpha > n$ . **There is  $c_n > 0$**  such that for any polynomial  $f$ , the following estimates hold:

- if  $V \in \mathfrak{G}^\alpha$ , then  $\sup_{t_0 \in [0,1]} \left\| \frac{d^n}{dt^n} f(H + tV) \Big|_{t=t_0} \right\|_{\frac{\alpha}{n}} \leq c_n \|V\|_\alpha^n \|f^{(n)}\|_{L_\infty(\mathbb{T})}$  ;
- if  $V \in \mathfrak{G}^n$ , then  $\sup_{t_0 \in [0,1]} \left| \operatorname{tr} \left( \frac{d^n}{dt^n} f(H + tV) \Big|_{t=t_0} \right) \right| \leq c_n \cdot \|V\|_n^n \cdot \|f^{(n)}\|_{L_\infty(\mathbb{T})}$ .

- The two cases above are the ones of self-adjoints and unitaries, while the case of contractions reduces to the case of unitaries by applying the **Sz.-Nagy-Foiaş dilation theory**.
- However, the proofs can not be carried over from the self-adjoint case and **require an independent treatment** for the case of unitaries.

# Advanced estimates of higher order in case of contractions

- The following results lies **at the core of the proof** of Theorem above.

Theorem (D. Potapov, A. Skripka & F.S., London Math. Soc. (to appear))

Let  $H$  and  $V$  be such that  $H$  and  $H + V$  are **contractions** and let  $n > 1$  and  $\alpha > n$ . **There is  $c_n > 0$**  such that for any polynomial  $f$ , the following estimates hold:

- if  $V \in \mathfrak{G}^\alpha$ , then  $\sup_{t_0 \in [0,1]} \left\| \frac{d^n}{dt^n} f(H + tV) \Big|_{t=t_0} \right\|_{\frac{\alpha}{n}} \leq c_n \|V\|_\alpha^n \|f^{(n)}\|_{L_\infty(\mathbb{T})}$  ;
- if  $V \in \mathfrak{G}^n$ , then  $\sup_{t_0 \in [0,1]} \left| \text{tr} \left( \frac{d^n}{dt^n} f(H + tV) \Big|_{t=t_0} \right) \right| \leq c_n \cdot \|V\|_n^n \cdot \|f^{(n)}\|_{L_\infty(\mathbb{T})}$  .

- The two cases above are the ones of self-adjoints and unitaries, while the case of contractions reduces to the case of unitaries by applying the **Sz.-Nagy-Foiaş dilation theory**.
- However, the proofs can not be carried over from the self-adjoint case and **require an independent treatment** for the case of unitaries.

# Advanced estimates of higher order in case of contractions

- The following results lies **at the core of the proof** of Theorem above.

Theorem (D. Potapov, A. Skripka & F.S., London Math. Soc. (to appear))

Let  $H$  and  $V$  be such that  $H$  and  $H + V$  are **contractions** and let  $n > 1$  and  $\alpha > n$ . **There is  $c_n > 0$**  such that for any polynomial  $f$ , the following estimates hold:

- if  $V \in \mathfrak{G}^\alpha$ , then  $\sup_{t_0 \in [0,1]} \left\| \frac{d^n}{dt^n} f(H + tV) \Big|_{t=t_0} \right\|_{\frac{\alpha}{n}} \leq c_n \|V\|_\alpha^n \|f^{(n)}\|_{L_\infty(\mathbb{T})}$  ;
- if  $V \in \mathfrak{G}^n$ , then  $\sup_{t_0 \in [0,1]} \left| \text{tr} \left( \frac{d^n}{dt^n} f(H + tV) \Big|_{t=t_0} \right) \right| \leq c_n \cdot \|V\|_n^n \cdot \|f^{(n)}\|_{L_\infty(\mathbb{T})}$  .

- The two cases above are the ones of self-adjoints and unitaries, while the case of contractions reduces to the case of unitaries by applying the **Sz.-Nagy-Foiaş dilation theory**.
- However, the proofs can not be carried over from the self-adjoint case and **require an independent treatment** for the case of unitaries.

# Advanced estimates of higher order in case of contractions

- The following results lies **at the core of the proof** of Theorem above.

Theorem (D. Potapov, A. Skripka & F.S., London Math. Soc. (to appear))

Let  $H$  and  $V$  be such that  $H$  and  $H + V$  are **contractions** and let  $n > 1$  and  $\alpha > n$ . **There is  $c_n > 0$**  such that for any polynomial  $f$ , the following estimates hold:

- if  $V \in \mathfrak{G}^\alpha$ , then  $\sup_{t_0 \in [0,1]} \left\| \frac{d^n}{dt^n} f(H + tV) \Big|_{t=t_0} \right\|_{\frac{\alpha}{n}} \leq c_n \|V\|_\alpha^n \|f^{(n)}\|_{L_\infty(\mathbb{T})}$  ;
- if  $V \in \mathfrak{G}^n$ , then  $\sup_{t_0 \in [0,1]} \left| \text{tr} \left( \frac{d^n}{dt^n} f(H + tV) \Big|_{t=t_0} \right) \right| \leq c_n \cdot \|V\|_n^n \cdot \|f^{(n)}\|_{L_\infty(\mathbb{T})}$  .

- The two cases above are the ones of self-adjoints and unitaries, while the case of contractions reduces to the case of unitaries by applying the **Sz.-Nagy-Foiaş dilation theory**.
- However, the proofs can not be carried over from the self-adjoint case and **require an independent treatment** for the case of unitaries.

# Applications and Connections, (aka Names dropping)

- Scattering theory [Birman, Krein, *Soviet Math. Dokl.* '62]:  
Krein's SSF = scattering phase
- Perturbation theory (connection with Fredholm perturbation determinant).
- More general perturbations have been studied:

$$H = (-\Delta)^{\frac{n}{4}+\epsilon}, \quad \epsilon > 0,$$

where  $V$  is a multiplication by a function in  $L^\infty(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$  (e.g., Koplienko, Yafaev, Azamov, Potapov, Skripka, F.S.).

- Inverse spectral problems for Schrödinger operators  $-\Delta + V$ , reconstruction of potentials from spectral data (e.g., Gesztesy, Simon, *Acta* '96)

- Integrated density of states for some random operators (e.g., Combes, Hislop, Nakamura, *CMP* '01)
- (Physics) multichannel scattering problem and physical calculations for neutron scattering off heavy nuclei (e.g., Rubtsova, Kukulin, Pomerantsev, Faessler, *Physical Review C* '10)
- Noncommutative geometry (e.g., Azamov, A.L. Carey, & F. S., *CMP* '07)  
Krein's SSF = spectral flow (provided both exist)
- Super-symmetric quantum systems and connection with Witten index (Gesztesy, Tomilov, Carey, Potapov, F.S.)
- Q: what is a geometric meaning of Koplienko's SSF?