ON A TRACE FORMULA FOR FUNCTIONS OF NONCOMMUTING OPERATORS

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ABSTRACT. The main result of the paper is that the Lifshits–Krein trace formula cannot be generalized to the case of functions of noncommuting self-adjoint operators. To prove this, we show that for pairs \((A_1, B_1)\) and \((A_2, B_2)\) of bounded self-adjoint operators with trace class differences \(A_2 - A_1\) and \(B_2 - B_1\), it is impossible to estimate the modulus of the trace of the difference \(f(A_2, B_2) - f(A_1, B_1)\) in terms of the norm of \(f\) in the Lipschitz class.

1. Introduction

The trace formula for functions of self-adjoint operators and the notion of spectral shift function appeared in the paper [L] by physicist I.M. Lifshits in connection with problems of quantum statistics and crystals theory. Later M.G. Krein in [Kr1] (see also his papers [Kr2] and [Kr3]) considered a significantly more general situation, extended the Lifshits result to the case of arbitrary self-adjoint operators with trace class difference, gave a mathematically rigorous definition of the spectral shift function and gave a mathematically rigorous proof of the trace formula.

Well then, let \((A_1, A_2)\) be a pair of (not necessarily bounded) self-adjoint operators with trace class difference. We refer the reader to the books [GK] and [BS2] for information on the trace class \(S_1\) and, on particular, on the linear functional trace on this class. For such a pair, there exists a unique integrable function \(\xi\) on the real line (called the spectral shift function of the pair \((A_1, A_2)\) ) such that

\[
\text{trace} \left( f(A_2) - f(A_1) \right) = \int_{\mathbb{R}} f'(t)\xi(t) \, dt \tag{1.1}
\]

for every sufficiently nice function \(f\). For example, one can take for \(f\) a rational function with poled off the real. Note that the Krein approach is based on perturbation determinants.

Next, M.G. Krein showed that the trace formula can be extended to the class of functions \(f\) whose derivative is the Fourier transform of a finite Borel measure on \(\mathbb{R}\). He also observed that the right-hand side of the equality is well-defined for an arbitrary Lipschitz function \(f\), i.e., for a function satisfying the inequality \(|f(x) - f(y)|\)
In this connection he posed the question of whether trace formula (1.1) can be extended to the class of arbitrary Lipschitz function $f$. Krein also posed in [Kr1] the problem to describe the maximal class of functions $f$, for which trace formula (1.1) holds for arbitrary pairs of self-adjoint operators with trace class difference.

It turned out, however that the answer to Krein’s question is negative. Indeed, Yu.B. Farforovskaya constructed in [F2] an example of a Lipschitz function $f$ on $\mathbb{R}$ and self-adjoint operators $A_1$ and $A_2$ with trace class difference such that $f(A_2) - f(A_1) \notin S_1$.

As for the Krein problem of describing the maximal class of functions, for which the Lifshitz–Krein trace formula is valid, it remained open for over 60 years and was solved in [Pe3]. It turned out (see [Pe3]) that the maximal class in question coincides with the class of operator Lipschitz functions. Recall that a function $f$ on $\mathbb{R}$ is called operator Lipschitz if the inequality

$$\|f(A) - f(B)\| \leq \text{const} \|A - B\|$$

holds for arbitrary self-adjoint operators $A$ and $B$ (no matter, bounded or unbounded). We refer the reader to the survey [AP] for detailed information on operator Lipschitz functions. In particular, formula (1.1) holds for functions $f$ in the homogeneous Besov class $B_{1,1}^1(\mathbb{R})$ which was proved earlier in [Pe1] and [Pe2].

Recall that it was shown in [F1] that not all Lipschitz functions are operator Lipschitz, while in [Mc] and [Ka] it was established that the function $x \mapsto |x|$ is not operator Lipschitz.

Let us also mention that in [BS1] an attempt was undertaken to obtain trace formula (1.1) with the help of double operator integrals. Using their approach, the authors of [BS1] managed to prove that for each pair $(A_1, A_2)$ of self-adjoint operator with trace class difference, there exists a finite real Borel measure $\nu$ on $\mathbb{R}$ (which can be called the spectral shift measure) such that

$$\text{trace} \left( f(A_2) - f(A_1) \right) = \int_{\mathbb{R}} f'(t) d\nu(t) \quad (1.2)$$

for sufficiently nice functions $f$. Clearly, it follows from Krein’s theorem that the measure $\nu$ is absolutely continuous with respect to Lebesgue measure $m$ and $d\nu = \xi dm$.

The program to obtain the full strength Krein theorem with the help of double operator integrals was realized in the recent paper [MNP]. To achieve this, the authors of [MNP] had to consider the problem of getting a trace formula for functions of contractions. It turned out that the absolute continuity of the spectral shift measure can be deduced from the Sz.-Nagy–Foiaş theorem on the absolute continuity of the spectral measure of the minimal unitary dilation of a completely nonunitary contraction (see [SNF]).

We also mention the paper [PSZ] in which a purely real method to prove the Krein theorem is given.

We would like to draw the reader’s attention to the fact that trace formula (1.1) (and even its weakened version (1.2)) implies the estimate

$$|\text{trace} \left( f(A_2) - f(A_1) \right)| \leq \text{const} \|f\|_{\text{Lip}}$$

for nice functions $f$, where $\|f\|_{\text{Lip}}$ is the (semi)norm of the function $f$ in the space of Lipschitz functions. However, as follows from the result of [F2] mentioned above, it is
impossible to replace the modulus of the trace with the trace norm of the difference $f(A_2) - f(A_1)$ on the left-hand side of this inequality.

In this paper we work on the problem of whether one can obtain an analogue of trace formula (1.1) for functions of pairs of noncommuting self-adjoint operators. Such functions of operators can be defined as double operator integrals

$$f(A, B) = \int_{\mathbb{R}^2} f(s, t) dE_A(s) dE_B(t)$$

where $E_A$ and $E_B$ are the spectral measures of the operators $A$ and $B$, see [ANP]. Recall that it was shown in [ANP] that under the assumption $1 \leq p \leq 2$, for functions $f$ in the homogeneous Besov class $B^{1, \infty}_\infty(\mathbb{R}^2)$ the following Lipschitz type estimate

$$\|f(A_2, B_2) - f(A_1, B_1)\| \leq \text{const} \|f\|_{B^{1, \infty}_\infty} \max\{\|A_2 - A_1\|_{\mathcal{S}_p}, \|B_2 - B_1\|_{\mathcal{S}_p}\}$$

holds for arbitrary pairs $(A_1, B_1)$ and $(A_2, B_2)$ of bounded self-adjoint operators such that $A_2 - A_1$ and $B_2 - B_1$ belong to the trace class $\mathcal{S}_p$. In particular, this is true for $p = 1$.

A question arises in a natural way of whether there is an analogue of trace formula (1.1) for functions of pairs of noncommuting operators. More precisely, let $(A_1, A_2)$ and $(B_1, B_2)$ be pairs of not necessarily commuting self-adjoint operators such that $A_2 - A_1$ and $B_2 - B_1$ belong to the trace class $\mathcal{S}_p$. Is it true that there exist integrable functions $\xi_1$ and $\xi_2$ on $\mathbb{R}^2$ such that

$$\text{trace} (f(A_2, B_2) - f(A_1, B_1)) = \int_{\mathbb{R}^2} \frac{\partial f}{\partial x}(x, y) \xi_1(x, y) \, dx \, dy$$

$$+ \int_{\mathbb{R}^2} \frac{\partial f}{\partial y}(x, y) \xi_2(x, y) \, dx \, dy$$

for sufficiently nice functions $f$, for example, for functions $f$ of class $B^{1, \infty}_\infty(\mathbb{R}^2)$?

If this is not true, is it still possible to obtain a weaker result, i.e., to generalize trace formula (1.2)? In other words, under the same hypotheses on the pairs of operators, do there exist finite Borel measures $\nu_1$ and $\nu_2$ such that the formula

$$\text{trace} (f(A_2, B_2) - f(A_1, B_1)) = \int_{\mathbb{R}^2} \frac{\partial f}{\partial x}(x, y) \, d\nu_1(x, y) + \int_{\mathbb{R}^2} \frac{\partial f}{\partial y}(x, y) \, d\nu_2(x, y)$$

holds for sufficiently nice functions $f$?

Note that each of the above formulae would imply the following estimate for the trace:

$$|\text{trace} (f(A_2, B_2) - f(A_1, B_1))| \leq \text{const} \|f\|_{\text{Lip}}.$$ 

In Section 3 of this paper we show that all these statements for functions of noncommuting self-adjoint operators are false.

2. Operator Lipschitz functions and perturbation by trace class operators
In this section we remind properties of operator Lipschitz functions that will be used in this paper. A function $f$ defined on an interval $J$ of the real line is called operator Lipschitz if the inequality
\[ \|f(A) - f(B)\| \leq \text{const} \|A - B\| \]
holds for arbitrary self-adjoint operators $A$ and $B$ with spectra in $J$.

First of all, we remind that operator Lipschitz functions on an interval $J$ are necessarily differentiable everywhere on $J$. This was established in [JW], see also the survey [AP]. However, as shown in [KS], they do not have to be continuously differentiable, see also the survey [AP].

We need the following result on the behavior of functions of operators under trace class perturbations:

**Theorem on trace class perturbations.** Let $J$ be an interval of the real line and let $f$ be a continuous function on $J$. The following are equivalent:

(a) $f$ is operator Lipschitz;
(b) the following inequality holds
\[ \|f(A) - f(B)\|_{S_1} \leq \text{const} \|A - B\|_{S_1} \]
for arbitrary self-adjoint operators $A$ and $B$ with spectra in $J$ and trace class difference $A - B$.
(c) $f(A) - f(B) \in S_1$, whenever $A$ and $B$ are not necessarily bounded self-adjoint operators with difference $A - B$ in $S_1$ and spectra in $J$.

Moreover, if $f$ is not operator Lipschitz, then for each positive number $\varepsilon$, there exist self-adjoint operators $A_{1,j}$ and $A_{2,j}$ whose spectra are contained in $\{x \in \mathbb{R} : |x - 2^{-j}| \leq 2^{-j-3}\}$ and such that
\[ A_{2,j} - A_{1,j} \in S_1, \quad \|A_{2,j} - A_{1,j}\|_{S_1} < 2^{-j} \text{ but } f(A_{2,j}) - f(A_{1,j}) \notin S_1 \]
(see §3).

3. The main result

The main purpose of this section is to show that analogues of the Lifshits–Krein trace formula for pairs of not necessarily commuting self-adjoint operators that were discussed in the introduction do not hold.

Let $j$ be a positive integer. Consider a real-valued function $\xi_j$ on $\mathbb{R}$ such that
\[ \xi_j(x) = \begin{cases} |x - 2^{-j}|, & |x - 2^{-j}| \leq 2^{-j-3}, \\ 0, & |x - 2^{-j}| \geq 2^{-j-2} \end{cases} \]
and such that $\xi_j \in C^\infty(\mathbb{R} \setminus \{2^{-j}\})$ and $\|\xi_j\|_{\text{Lip}} \leq \text{const}$. By the Johnson–Williams theorem (see §2), the function $\xi_j$ is not operator Lipschitz, and so there exist self-adjoint operators $A_{1,j}$ and $A_{2,j}$ whose spectra are contained in $\{x \in \mathbb{R} : |x - 2^{-j}| \leq 2^{-j-3}\}$ and such that
\[ A_{2,j} - A_{1,j} \in S_1, \quad \|A_{2,j} - A_{1,j}\|_{S_1} < 2^{-j} \text{ but } \xi_j(A_{2,j}) - \xi_j(A_{1,j}) \notin S_1 \]
It follows that we can uniformly approximate the function $\xi_j$ by an infinitely smooth real-valued function $\psi_j$ such that

$$\text{supp } \psi_j \subset \{ x \in \mathbb{R} : |x - 2^{-j}| \leq 2^{-j-3} \},$$

$$\|\psi_j\|_{\text{Lip}} \leq 2^j |\xi_j|_{\text{Lip}} \text{ and } \|\psi_j(A_{2,j}) - \psi_j(A_{1,j})\|_{S_1} \geq 1.$$

Consider the self-adjoint operator $Q_j \overset{\text{def}}{=} \psi_j(A_{2,j}) - \psi_j(A_{1,j})$ and let $E_j$ be its spectral measure. Let $B_j$ be the self-adjoint (and unitary at the same time!) operator, which coincides with the identity operator $I$ on the subspace $E_j((0, \infty))$ and coincides with the operator $-I$ on the subspace $E_j((\infty, 0))$. Then, obviously, the operator $(\psi_j(A_{2,j}) - \psi_j(A_{1,j}))B_j$ is nonnegative and

$$\text{trace } ((\psi_j(A_{2,j}) - \psi_j(A_{1,j}))B_j) = \|\psi_j(A_{2,j}) - \psi_j(A_{1,j})\|_{S_1}.$$

Let us define now the operators $A_1$, $A_2$ and $B$ as the orthogonal sums:

$$A_1 = \bigoplus_{j \geq 1} A_{1,j}, \quad A_2 = \bigoplus_{j \geq 1} A_{2,j}, \quad \text{and } B = \bigoplus_{j \geq 1} B_j.$$

Clearly, $A_2 - A_1 \in S_1$ and

$$\|A_2 - A_1\|_{S_1} = \sum_{j \geq 1} \|A_{2,j} - A_{1,j}\|_{S_1} \leq 1.$$

**Theorem 3.1.** Let $A_1$, $A_2$ and $B$ be the self-adjoint operators defined above. There are no complex Borel measures $\nu_1$ and $\nu_2$ such that the trace formula

$$\text{trace } (f(A_2, B) - f(A_1, B)) = \int_{\mathbb{R}^2} \left( \frac{\partial f(x, y)}{\partial x} \ d\nu_1(x, y) \right)$$

$$+ \int_{\mathbb{R}^2} \left( \frac{\partial f(x, y)}{\partial y} \ d\nu_2(x, y) \right) \quad (3.1)$$

holds for an arbitrary infinitely smooth function $f$ with compact support.

**Proof.** For a positive integer $n$, we define the infinitely smooth function $\varphi_n$ on $\mathbb{R}$ by

$$\varphi_n = \sum_{j=1}^{n} \psi_j,$$

where the $\psi_j$ are the functions constructed above. It follows easily from the definition of $\psi_j$ that $\|\varphi_n\|_{\text{Lip}} \leq \text{const}$. Consider an infinitely smooth function $\phi$ on $\mathbb{R}$ such that $\phi(y) = y$ for $y$ in $[-1, 1]$ and $\text{supp } \phi \subset [-2, 2]$. Finally, we define the function $f_n$ on $\mathbb{R}^2$ by

$$f_n(x, y) = \varphi_n(x)\phi(y), \quad (x, y) \in \mathbb{R}^2.$$

Clearly, the function $f_n$ is infinitely smooth, has compact support and $\|f_n\|_{\text{Lip}} \leq \text{const}$. If such measures $\nu_1$ and $\nu_2$ existed, equality $(3.1)$ would imply that

$$|\text{trace } f_n(A_2, B) - f_n(A_1, B)| \leq \text{const } \|f_n\|_{\text{Lip}} \leq \text{const}.$$
However, it is easy to see that
\[
\text{trace} \left( f_n(A_2, B) - f_n(A_1, B) \right) = \sum_{j=1}^{n} \text{trace} \left( (\psi_j(A_{2,j}) - \psi_j(A_{1,j}))B_j \right)
\]
\[
= \sum_{j=1}^{n} \|\psi_j(A_{2,j}) - \psi_j(A_{1,j})\|_{S_1} \geq n.
\]

We get a contradiction. ■

4. Open problems

1. Estimates of the moduli of traces. We have mentioned in the introduction that in the case of functions of a single self-adjoint operator, the modulus of the trace of the difference \(f(A) - f(B)\) admits a considerably stronger estimate than the trace norm \(\|f(A) - f(B)\|_{S_1}\). A natural question arises of whether the same can be said in the case of functions of two noncommuting self-adjoint operators. It would be interesting to obtain a kind of an optimal estimate for \(\|\text{trace} (f(A_2, B) - f(A_1, B))\|\). This could lead to finding a version of a trace formula.

2. A trace formula for functions of normal operators. In §3 of this paper we have shown that the Lifshits–Krein trace formula (1.1) cannot be generalized to the case of pairs of noncommuting self-adjoint operators. What is the situation in the case of functions of pairs of commuting self-adjoint operators?

Clearly, it is the same as to consider functions of normal operators. Recall that in the paper [APPS] it was shown that the inequality
\[
\| (f(N_2) - f(N_1)) \|_{S_p} \leq \text{const} \|f\|_{B^1_{\infty,1}} \|N_2 - N_1\|_{S_p}
\]
holds for any function \(f\) of Besov class \(B^1_{\infty,1}(\mathbb{R}^2)\) and for any \(p\) in \([1, \infty)\); moreover, the constant does not depend on \(p\).

The question is the following: let \(N_1\) and \(N_2\) be normal operators on Hilbert space. Is it true that there exist finite Borel measures \(\nu_1\) and \(\nu_2\) such that the trace formula
\[
\text{trace} \left( f(N_2) - f(N_1) \right) = \int_{\mathbb{R}^2} \frac{\partial f}{\partial x}(x, y) d\nu_1(x, y) + \int_{\mathbb{R}^2} \frac{\partial f}{\partial y}(x, y) d\nu_2(x, y)
\]
holds for sufficiently smooth functions \(f\) on \(\mathbb{R}^2\)? Note that if the answer to this question is positive, then for such normal operators \(N_1\) and \(N_2\) the inequality
\[
\| \text{trace} (f(N_2) - f(N_1)) \| \leq \text{const} \|f\|_{\text{Lip}}
\]
holds for sufficiently nice functions \(f\) on \(\mathbb{R}^2\). In any case, it would be important to find out whether under the above assumptions on \(f\) can estimate \(\| \text{trace} (f(N_2) - f(N_1)) \|\) better than \(\| (f(N_2) - f(N_1)) \|_{S_1}\).

If the above question has an affirmative answer, it is natural to ask the question of whether one can select measures \(\nu_1\) and \(\nu_2\) to be absolutely continuous with respect to Lebesgue measure on \(\mathbb{R}^2\).
3. A trace formula for functions of commuting self-adjoint operators. It was shown in [NP] that if \((A_1, A_2, \ldots, A_n)\) and \((B_1, B_2, \ldots, B_n)\) are collections of commuting self-adjoint operators such that \(B_j - A_j \in S_p, 1 \leq j \leq n,\) and \(1 \leq p \leq \infty,\) then
\[
\|f(B_1, \ldots, B_n) - f(A_1, \ldots, A_n)\|_{S_p} \leq C \max_{1 \leq j \leq n} \|B_j - A_j\|_{S_p}
\]
for every function \(f\) of Besov class \(B^1_{\infty,1}(\mathbb{R}^n)\).

In the case when the question posed in Subsection 2 has an affirmative answer, it would be interesting to find out whether one can generalize the Lifshits–Krein trace formula (1.1) to the case of collections of commuting self-adjoint operators.

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