THE LIFSHITS–KREIN TRACE FORMULA AND OPERATOR LIPSCHITZ FUNCTIONS

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ABSTRACT. We describe the maximal class of functions f on the real line, for which the Lifshitz–Krein trace formula $\operatorname{trace}(f(A)-f(B))=\int_{\mathbb{R}} f'(s)\boldsymbol{\xi}(s)\,ds$ holds for arbitrary self-adjoint operators A and B with $A-B$ in the trace class $\boldsymbol{S}_1$. We prove that this class of functions coincide with the class of operator Lipschitz functions.

CONTENTS

1. Introduction

The purpose of this paper is to describe the class functions, for which the Lifshitz–Krein trace formula holds. The Lifshitz–Krein trace formula plays a significant role in perturbation theory. It was discovered by Lifshits [L] in a special case and by Krein [Kr] in the general case. This formula allows one to compute the trace of the difference $f(A)-f(B)$ of a function f of an unperturbed self-adjoint operator A and a perturbed self-adjoint operator B provided the perturbation $B-A$ belongs to trace class $\boldsymbol{S}_1$. M.G. Krein proved that for each such pair there exists a unique function $\boldsymbol{\xi}$ in $L^1(\mathbb{R})$ such that for every function f whose derivative is the Fourier transform of and L^1 function, the operator $f(A)-f(B)$ belongs to $\boldsymbol{S}_1$ and the following trace formula holds:

$$\operatorname{trace}\big(f(A)-f(B)\big)=\int_{\mathbb{R}} f'(s)\boldsymbol{\xi}(s)\,ds \tag{1.1}$$

the author is partially supported by NSF grant DMS 1300924.

(see [Kr]). The function $\boldsymbol{\xi}$ is called the *spectral shift function associated with the pair* (A, B). Clearly, the right-hand side of (1.1) makes sense for arbitrary Lipschitz function f. In this connection Krein asked the question of whether it is true that for an arbitrary Lipschitz function f, the operator $f(A) - f(B)$ is in $\boldsymbol{S}_1$ and trace formula (1.1) holds. *It turns out that this is false.* In [F] Farforovskaya gave an example of self-adjoint operators A and B with $A - B \in \boldsymbol{S}_1$ and a Lipschitz function f such that $f(A) - f(B) \notin \boldsymbol{S}_1$.

Later it was shown in [Pe2] and [Pe3] that formula (1.1) holds, whenever A and B are self-adjoint operators with $A - B \in \boldsymbol{S}_1$ and f belongs to the Besov space $B^1_{\infty,1}(\mathbb{R})$ (we refer the reader to [Pee] and [Pe4] for an introduction to Besov classes). Necessary conditions are also obtained in [Pe2] and [Pe3]. In particular, it was shown in [Pe2] and [Pe3] that if $f(A) - f(B) \in \boldsymbol{S}_1$ whenever A and B are self-adjoint operators with $A - B \in \boldsymbol{S}_1$, then f locally belongs to the Besov space $B^1_{1,1}(\mathbb{R})$. Note that those necessary conditions were deduced from the description of trace class Hankel operators [Pe1] (see also [Pe4]).

The main objective of this paper is to describe the class of functions f, for which trace formula (1.1) holds for arbitrary self-adjoint operators A and B with $A - B \in \boldsymbol{S}_1$.

It is well known (see e.g. [AP2]) that for a function f on $\mathbb{R}$, the following properties are equivalent:

(i) *there exists a positive number C such that*

$$\|f(A) - f(B)\| \le C\|A - B\| \tag{1.2}$$

for all bounded self-adjoint operators A and B;

(ii) *there exists a positive number C such that inequality* (1.2) *holds, whenever A and B are (not necessarily bounded) self-adjoint operators such that $A - B$ is bounded;*

(iii) *there exists a positive number C such that*

$$\|f(A) - f(B)\|_{\boldsymbol{S}_1} \le C\|A - B\|_{\boldsymbol{S}_1} \tag{1.3}$$

for all bounded self-adjoint operators A and B with $A - B \in \boldsymbol{S}_1$;

(iv) *there exists a positive number C such that inequality* (1.3) *holds,, whenever A and B are (not necessarily bounded) self-adjoint operators such that $A - B \in \boldsymbol{S}_1$;*

(v) *$f(A) - f(B) \in \boldsymbol{S}_1$, whenever A and B are (not necessarily bounded) self-adjoint operators such that $A - B \in \boldsymbol{S}_1$.*

Note that the minimal value of the constant C is the same in (i)–(iv).

Functions satisfying (i) are called *operator Lipschitz*. We denote by $\mathrm{OL}(\mathbb{R})$ the space of operator Lipschitz functions on $\mathbb{R}$. For $f \in \mathrm{OL}(\mathbb{R})$, we define its quasi norm $\|f\|_{\mathrm{OL}}$ as the infimum of all constants C, for which inequality (1.2) holds. In other words,

$$\|f\|_{\mathrm{OL}} = \sup\left\{\frac{\|f(A) - f(B)\|_{\boldsymbol{S}_1}}{\|A - B\|_{\boldsymbol{S}_1}} : \ A \ \text{ and } \ B \ \text{ are self-adjoint, } \ A - B \ \text{ is bounded}\right\}$$

$$= \sup\left\{\frac{\|f(A) - f(B)\|}{\|A - B\|} : \ A \ \text{ and } \ B \ \text{ are self-adjoint, } \ A - B \in \boldsymbol{S}_1\right\}.$$

It was shown in [JW] that operator Lipschitz functions are differentiable everywhere on $\mathbb{R}$. Note that this implies that the function $x \mapsto |x|$ is not operator Lipschitz, the fact established earlier in [Mc] and [Ka]. On the other hand, an operator Lipschitz function does not have to be continuously differentiable; in particular, the function $x \mapsto x^2 \sin x^{-1}$ is operator Lipschitz, see [KS].

For a differentiable function f on $\mathbb{R}$, we consider the divided difference $\mathfrak{D}f$ defined by

$$(\mathfrak{D}f)(x,y) = \begin{cases} \frac{f(x)-f(y)}{x-y}, & x \neq y \\ f'(x), & x = y. \end{cases} \tag{1.4}$$

It turns out (see e.g., [AP2]) that a differentiable function on $\mathbb{R}$ is operator Lipschitz if and only if the divided difference $\mathfrak{D}f$ is a Schur multiplier (see § 2) for the definition.

The main purpose of this paper is to prove that *the condition* $f \in \mathrm{OL}(\mathbb{R})$ *is not only a necessary condition for the Lifshits–Krein trace formula* (1.1) *to hold for arbitrary self-adjoint operators* A *and* B *with* $A - B \in \boldsymbol{S}_1$*, but is also sufficient.* This will be proved in § 6.

In § 2 We define double operator integrals and Schur multipliers. In § 3 we state a result of [KPSS] on the differentiability of the function $t \mapsto f(A+tK) - f(A)$ in the Hilbert–Schmidt norm. We state a characterization of the space of Schur multipliers in terms of Haagerup tensor products in § 4. Finally, in § 5 we obtain a formula for the trace of double operator integrals.

2. **Double operator integrals and Schur multipliers**

Double operator integrals appeared in the paper [DK] by Daletskii and S.G. Krein. Later the beautiful theory of double operator integrals was created by Birman and Solomyak in [BS1], [BS2], and [BS4].

Let $(\mathscr{X}, E_1)$ and $(\mathscr{Y}, E_2)$ be spaces with spectral measures E_1 and E_2 on a Hilbert space $\mathscr{H}$ and let Φ be a bounded measurable function on $\mathscr{X} \times \mathscr{Y}$. Double operator integrals are expressions of the form

$$\int\limits_{\mathscr{X}}\int\limits_{\mathscr{Y}} \Phi(x,y)\, dE_1(x) T\, dE_2(y). \tag{2.1}$$

Birman and Solomyak starting point is the case when T belongs to the Hilbert–Schmidt class $\boldsymbol{S}_2$. For a bounded measurable function on Φ on $\mathscr{X} \times \mathscr{Y}$ and an operator T of class $\boldsymbol{S}_2$, consider the spectral measure $\mathscr{E}$ whose values are orthogonal projections on the Hilbert space $\boldsymbol{S}_2$, which is defined by

$$\mathscr{E}(Ł \times \Delta)T = E_1(Ł) T E_2(\Delta), \quad T \in \boldsymbol{S}_2,$$

Ł and Δ being measurable subsets of $\mathscr{X}$ and $\mathscr{Y}$. It was shown in [BS5] that $\mathscr{E}$ extends to a spectral measure on $\mathscr{X} \times \mathscr{Y}$. For a bounded measurable function Φ on $\mathscr{X} \times \mathscr{Y}$, the double operator integral (2.1) is defined by

$$\int\limits_{\mathscr{X}}\int\limits_{\mathscr{Y}} \Phi(x,y)\, dE_1(x) T\, dE_2(y) \stackrel{\mathrm{def}}{=} \left(\int\limits_{\mathscr{X}\times\mathscr{Y}} \Phi\, d\mathscr{E} \right) T.$$

Clearly,

$$\left\|\int\limits_{\mathscr{X}}\int\limits_{\mathscr{Y}}\Phi(x,y)\,dE_1(x)T\,dE_2(y)\right\|_{\boldsymbol{S}_2}\le\|\Phi\|_{L^\infty}\|T\|_{\boldsymbol{S}_2}.$$

If

$$\int\limits_{\mathscr{X}}\int\limits_{\mathscr{Y}}\Phi(x,y)\,dE_1(x)T\,dE_2(y)\in\boldsymbol{S}_1$$

for every $T\in\boldsymbol{S}_1$, we say that Φ is a *Schur multiplier of* $\boldsymbol{S}_1$ *associated with the spectral measures* E_1 *and* E_2. *We denote by* $\mathfrak{M}(E_1,E_2)$ *the space of Schur multipliers of* $\boldsymbol{S}_1$ *with respect to* E_1 *and* E_2. The norm $\|\Phi\|_{\mathfrak{M}(E_1,E_2)}$ of Φ in the space $\mathfrak{M}(E_1,E_2)$ is, by definition, the norm of the linear transformer

$$T\mapsto\int\limits_{\mathscr{X}}\int\limits_{\mathscr{Y}}\Phi(x,y)\,dE_1(x)T\,dE_2(y)$$

on the class $\boldsymbol{S}_1$.

If $\Phi\in\mathfrak{M}(E_1,E_2)$, one can define by duality double operator integrals of the form (2.1) for an arbitrary bounded linear operator T. However, we do not need this in this paper.

We are going to discuss briefly in § 4 characterizations of Schur multipliers.

Birman and Solomyak proved in [BS4] that if f is a Lipschitz function and A and B are not necessarily bounded self-adjoint operators with $A-B\in\boldsymbol{S}_2$, then

$$f(A)-f(B)=\iint\limits_{\mathbb{R}\times\mathbb{R}}\frac{f(x)-f(y)}{x-y}\,dE_A(x)(A-B)\,dE_B(y).\tag{2.2}$$

Note that for an arbitrary Lischitz function f, the divided difference $\mathfrak{D}f$ is not always naturally defined on the diagonal. However, we can define $\mathfrak{D}f$ on the diagonal by an arbitrary bounded measurable function and the right-hand side of (2.2) does not depend on the values on the diagonal. It follows from (2.2) that

$$\|f(A)-f(B)\|_{\boldsymbol{S}_2}\le\|f\|_{\rm Lip}\|A-B\|_{\boldsymbol{S}_2},$$

where the Lipschitz (semi)norm $\|f\|_{\rm Lip}$ of f is, by definition,

$$\sup\left\{\frac{|f(x)-f(y)|}{|x-y|}:\ x,\ y\in\mathbb{R},\ x\ne y\right\}.$$

On the other hand, if A and B are not necessarily bounded self-adjoint operators with $A-B\in\boldsymbol{S}_1$ and f is an operator Lipschitz function, then

$$f(A)-f(B)=\iint\limits_{\mathbb{R}\times\mathbb{R}}\big(\mathfrak{D}f\big)(x,y)\,dE_A(x)(A-B)\,dE_B(y).\tag{2.3}$$

(see [BS4]). Here the divided difference $\mathfrak{D}f$ is defined by (1.4). It follows from (2.3) that

$$\|f(A)-f(B)\|_{\boldsymbol{S}_1}\le\|f\|_{\rm OL}\|A-B\|_{\boldsymbol{S}_1}.$$

3. **Differentiability in the Hilbert–Schmidt norm**

Suppose that A and B are not necessarily bounded self-adjoint operators on Hilbert space such that $A-B\in \boldsymbol{S}_2$. Consider the parametric family A_t, $0\le t\le 1$, defined by $A_t=A+tK$, where $K\stackrel{\mathrm{def}}{=}B-A$. We need the following result of [KPSS], Theorem 7.18:

Suppose that f is a Lipschitz function on $\mathbb{R}$ that is differentiable at every point of $\mathbb{R}$. Then the function $s\mapsto f(A_s)-f(A)$ is differentiable on $[0,1]$ in the Hilbert–Schmidt norm and

$$\frac{d}{ds}\big(f(A_s)-f(A)\big)\Big|_{s=t}=\iint\limits_{\mathbb{R}\times\mathbb{R}}(\mathfrak{D}f)(x,y)\,dE_t(x)K\,dE_t(y).$$

4. **Schur multipliers and Haagerup tensor products**

Let $(\mathscr{X},E_1)$ and $(\mathscr{Y},E_2)$ be spaces with spectral measures E_1 and E_2 on Hilbert space. There are several characterizations of the class $\mathfrak{M}(E_1,E_2)$ of Schur multipliers, see [Pe2], [Pi], [AP2]. We need the following characterization in terms of the Haagerup tensor product of L^∞ spaces:

Let Φ be a measurable function on $\mathscr{X}\times\mathscr{Y}$. Then $\Phi\in\mathfrak{M}(E_1,E_2)$ if and only if Φ belongs to the Haagerup tensor product $L^\infty(E_1)\otimes_{\mathrm{h}}L^\infty(E_2)$, i.e., Φ admits a representaion

$$\Phi(x,y)=\sum_n\varphi_n(x)\psi_n(y),$$

where $\varphi_n\in L^\infty(E_1)$, $\psi_n\in L^\infty(E_2)$, and

$$\sum_n|\varphi_n|^2\in L^\infty(E_1)\quad\text{and}\quad\sum_n|\psi_n|^2\in L^\infty(E_2).$$

Suppose now that E_1 and E_2 are Borel spectral measures on locally compact topological spaces X and Y. In this case the following result holds (see [AP2]):

Let Φ be a function on $\mathscr{X}\times\mathscr{Y}$ that is continuous in each variable. Then $\Phi\in\mathfrak{M}(E_1,E_2)$ if and only if it belongs to the Haagerup tensor product $C_{\mathrm{b}}(\mathscr{X})\otimes_{\mathrm{h}}C_{\mathrm{b}}(\mathscr{Y})$ of the spaces of bounded continuous functions on $\mathscr{X}$ and $\mathscr{Y}$, i.e., Φ admits a representation

$$\Phi(x,y)=\sum_n\varphi_n(x)\psi_n(y),$$

where $\varphi_n\in C_{\mathrm{b}}(\mathscr{X})$, $\psi_n\in C_{\mathrm{b}}(\mathscr{Y})$ and the functions

$$\sum_n|\varphi_n|^2\quad\textit{and}\quad\sum_n|\psi_n|^2$$

are bounded.

5. **The trace of double operator integrals**

Let T be a trace class operator on Hilbert space and let E be a spectral measure on a σ-algebra of subsets of a set $\mathscr{X}$. If Φ is a Schur multiplier, i.e., $\Phi \in \mathfrak{M}(E,E)$, then the double operator integral

$$\iint \Phi(x,y)\,dE(x)T\,dE(y)$$

belongs to $\boldsymbol{S}_1$. Let us compute its trace. In [BS4] the following trace formula was found:

$$\operatorname{trace}\left(\iint \Phi(x,y)\,dE(x)T\,dE(y)\right) = \int \Phi(x,x)\,d\mu(x), \tag{5.1}$$

where μ is the complex measure defined by

$$\mu(\Delta) = \operatorname{trace}\big(TE(\Delta)\big).$$

The problem is how we can interpret the function $x \mapsto \Phi(x,x)$ for functions Φ in $\mathfrak{M}(E,E)$. In [Pe5] the following justification of formula (5.1) was given. We can define the trace $\mathscr{T}\Phi$ of a function Φ in $\mathfrak{M}(E,E)$ on the diagonal by the formula

$$(\mathscr{T}\Phi)(x) \stackrel{\text{def}}{=} \sum_n \varphi_n(x)\psi_n(x),$$

where

$$\Phi(x,y) = \sum_n \varphi_n(x)\psi_n(y) \tag{5.2}$$

is a representation of Φ as an element of the Haagerup tensor product $L^\infty(E)\otimes_{\rm h} L^\infty(E)$, i.e.,

$$\sum_m |\varphi_n|^2 \in L^\infty(E) \quad \text{and} \quad \sum_m |\psi_n|^2 \in L^\infty(E). \tag{5.3}$$

Clearly, the trace of $\Phi \in \mathfrak{M}(E,E)$ on the diagonal belongs to $L^\infty(E)$. Then formula (5.1) holds if $\Phi(x,x)$ is understood as $(\mathscr{T}\Phi)(x)$, see [Pe5], § 1.1.

Suppose now that E is a Borel spectral measure on a locally compact topological space $\mathscr{X}$ and Φ is a function on $\mathscr{X}\times\mathscr{X}$ that is continuous in each variable. As we have mentioned in § 2, Φ admits a representation of the form (5.2), in which the functions φ_n and ψ_n satisfy (5.3) and are continuous functions on $\mathscr{X}$. It is easy to see that in this case $(\mathscr{T}\Phi)(x) = \Phi(x,x)$, $x \in \mathscr{X}$. In other words, the following theorem holds:

Theorem 5.1. *Let E be a spectral measure on a locally compact topological space $\mathscr{X}$. Suppose that Φ is a function of class $\mathfrak{M}(E,E)$. If Φ is continuous in each variable, then formula* (5.1) *holds for an arbitrary trace class operator T.*

6. **The Lifshits–Krein trace formula for arbitrary operator Lipschitz functions**

Suppose that A and B are self-adjoint operators on Hilbert space such that $A-B\in\boldsymbol{S}_1$. Let $\boldsymbol{\xi}$ be the spectral shift function associated with the pair (A,B). As we have mentioned in § 2, for an arbitrary operator Lipschitz function f on $\mathbb{R}$, the operator $f(A)-f(B)$ belongs to trace class. The following theorem is the main result of the paper.

Theorem 6.1. *Let $f\in\mathrm{OL}(\mathbb{R})$. Then*

$$\operatorname{trace}\big(f(A)-f(B)\big)=\int_{\mathbb{R}}f'(s)\boldsymbol{\xi}(s)\,ds.$$

To prove the theorem, we are going to use an approach of Birman and Solomyak in [BS3] to the Lifshits–Krein trace formula. In [BS3] they used their approach under more restrictive assumptions on f.

Proof. Obviously, f is a Lipschitz function. As we have mentioned in the introduction, f is a differentiable function at every point of $\mathbb{R}$ (but not necessarily continuously differentiable!). Put $K\stackrel{\mathrm{def}}{=}B-A$. Consider the parametric family $\{A_t\}_{0\le t\le 1}$, $A_t\stackrel{\mathrm{def}}{=}A+tK$. Then $A_0=A$ and $A_1=B$. The operator K obviously belongs to the Hilbert–Schmidt class $\boldsymbol{S}_2$. As we have mentioned in § 3, the function $t\mapsto f(A_t)-f(A)$ is differentiable in the Hilbert–Schmidt norm and

$$Q_t\stackrel{\mathrm{def}}{=}\frac{d}{ds}\big(f(A_s)-f(A)\big)\Big|_{s=t}=\iint\limits_{\mathbb{R}\times\mathbb{R}}\frac{f(x)-f(y)}{x-y}\,dE_t(x)K\,dE_t(y)\in\boldsymbol{S}_2,$$

where E_t is the spectral measure of A_t.

On the other hand, since the divided difference $\mathfrak{D}f$ is a Schur multiplier of of $\boldsymbol{S}_1$ (see the introduction), it follows that

$$Q_t\in\boldsymbol{S}_1,\quad 0\le t\le 1,\quad\text{and}\quad\sup_{t\in[0,1]}\|Q_t\|_{\boldsymbol{S}_1}<\infty.$$

We have

$$f(A)-f(B)=-\int_0^1Q_t\,dt,$$

where the integral on the right is understood in the sense of Bochner in the space $\boldsymbol{S}_1$. It follows that

$$\operatorname{trace}\big(f(A)-f(B)\big)=-\int_0^1\operatorname{trace}(Q_t)\,dt.$$

Since the function f is differentiable everywhere, the divided difference $\mathfrak{D}f$ is continuous in each variable. By Theorem 5.1,

$$\operatorname{trace}Q_t=\int_{\mathbb{R}}f'(x)\,d\nu_t(x),$$

where the signed measure ν_t is defined by

$$\nu_t(\Delta)\stackrel{\mathrm{def}}{=}\operatorname{trace}\big(E_t(\Delta)K\big)\quad\text{for a Borel subset}\quad\Delta\quad\text{of}\quad\mathbb{R}.$$

We identify here the space of complex Borel measures on $\mathbb{R}$ with the dual space to the Banach space of continuous functions on $\mathbb{R}$ with zero limit at infinity. Then the function $t \mapsto \nu_t$ is continuous in the weak-$*$ topology on the space of complex Borel measures. Indeed, if h is continuous on $\mathbb{R}$ and $\lim_{|x|\to\infty} h(x) = 0$, then

$$\int h\, d\nu_t = \operatorname{trace}\big(h(A_t)K\big).$$

The function $t \mapsto h(A_t)$ is a continuous function on $[0,1]$ in the operator norm; this follows from the fact that h is an operator continuous function (see [AP1], § 8). Thus the function $t \mapsto \operatorname{trace}\big(h(A_t)K\big)$ is continuous.

Therefore we can define the signed Borel measure ν on $\mathbb{R}$ by

$$\nu = \int_0^1 \nu_t\, dt.$$

It follows that

$$\operatorname{trace}\big(f(A) - f(B)\big) = -\int_{\mathbb{R}} f'\, d\nu.$$

On the other hand, for smooth functions g with compact support,

$$\operatorname{trace}\big(g(A) - g(B)\big) = \int_{\mathbb{R}} g' \boldsymbol{\xi}\, d\boldsymbol{m},$$

where $\boldsymbol{\xi}$ is the spectral shift function.

It follows that ν is absolutely continuous with respect to Lebesgue measure and $d\nu = -\boldsymbol{\xi} d\boldsymbol{m}$. ■

Theorem 6.1 implies the following result:

Theorem 6.2. *Let f be an operator Lipschitz function and let A and B be self-adjoint operators such that $A - B \in \boldsymbol{S}_1$. Then the function*

$$t \mapsto \operatorname{trace}\big(f(A - tI) - f(B - tI)\big), \quad t \in \mathbb{R},$$

is continuous on $\mathbb{R}$.

Proof. Consider the function f_t, $t \in \mathbb{R}$, defined by $f_t(x) \stackrel{\text{def}}{=} f(x - t)$. Let $\boldsymbol{\xi}$ be the spectral shift function associated with (A, B). It is easy to see that

$$\operatorname{trace}\big(f(A + tI) - f(B + tI)\big) = \operatorname{trace}\big(f_t(A) - f_t(B)\big) = \int_{\mathbb{R}} f'(x - t)\boldsymbol{\xi}(x)\, d\boldsymbol{m}(x),$$

which depends on t continuously. ■

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