

AN EXTENSION OF THE
KOPLIENKO-NEIDHARDT TRACE FORMULAE

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ABSTRACT. Koplienko [Ko1] found a trace formula for perturbations of self-adjoint operators by operators of Hilbert Schmidt class \mathcal{S}_2 . A similar formula in the case of unitary operators was obtained by Neidhardt [N]. In this paper we improve their results and obtain sharp conditions under which the Koplienko–Neidhardt trace formulae hold.

1. Introduction

The spectral shift function for a trace class perturbation of a self-adjoint (unitary) operator plays a very important role in perturbation theory. It was introduced in a special case by I.M. Lifshitz [L] and in the general case by M.G. Krein [Kr1]. He showed that for a pair of self-adjoint (not necessarily bounded) operators A and B satisfying $B - A \in \mathcal{S}_1$ there exists a unique function $\xi \in L^1(\mathbb{R})$ such that

$$\text{trace}(\varphi(B) - \varphi(A)) = \int_{\mathbb{R}} \varphi'(x)\xi(x) dt, \quad (1.1)$$

whenever φ is a function on \mathbb{R} with Fourier transform of φ' in $L^1(\mathbb{R})$. The function ξ is called the *spectral shift function corresponding to the pair* (A, B) . We use the notation \mathcal{S}_1 for the class of nuclear operators (trace class) on Hilbert space.

A similar result was obtained in [Kr2] for pairs of unitary operators (U, V) with $V - U \in \mathcal{S}_1$. For each such pair there exists a function ξ on the unit circle \mathbb{T} of class $L^1(\mathbb{T})$ such that

$$\text{trace}(\varphi(V) - \varphi(U)) = \int_{\mathbb{T}} \varphi'(\zeta)\xi(\zeta) d\mathbf{m}(\zeta), \quad (1.2)$$

whenever φ' has absolutely convergent Fourier series. (Throughout the paper \mathbf{m} is normalized Lebesgue measure on \mathbb{T} .) Such a function ξ is unique modulo a constant and it is called a *spectral shift function corresponding to the pair* (U, V) . We refer the reader to the lectures of M.G. Krein [Kr3], in which the above results were discussed in detail (see also the survey article [BY]).

Note that spectral shift function plays an important role in perturbation theory. We mention here the paper [BK], in which the following important formula was found:

$$\det S(x) = e^{-2\pi i\xi(x)},$$

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where S is the scattering matrix corresponding to the pair (A, B) ; see also the monograph [Y].

It was shown later in [BS3] that formulae (1.1) and (1.2) hold under less restrictive assumptions on φ .

Note that the right-hand sides of (1.1) and (1.2) make sense for an arbitrary Lipschitz function φ . However, it turns out that the condition $\varphi \in \text{Lip}$ (i.e., φ is a Lipschitz function) does not imply that $\varphi(B) - \varphi(A)$ or $\varphi(V) - \varphi(U)$ belong to \mathcal{S}_1 . This is not even true for bounded A and B and continuously differentiable φ . The first such examples were given in [F].

In [Pe1] and [Pe2] with the help of the nuclearity criterion for Hankel operators (see recent monograph [Pe4]) necessary conditions (in terms of Besov classes and Carleson measures) were found on φ for the operator $\varphi(B) - \varphi(A)$ (or $\varphi(V) - \varphi(U)$) to belong to \mathcal{S}_1 . Those necessary conditions also imply that the condition $\varphi \in C^1$ is not sufficient for those operators to be in \mathcal{S}_1 (even for bounded A and B).

In the same papers [Pe1] and [Pe2] sharp sufficient conditions were found. It was shown in [Pe1] that if φ is a function on \mathbb{T} of Besov class $B_{\infty 1}^1$, then trace formula (1.2) holds. Similarly, it was shown in [Pe2] that if φ is a function on \mathbb{R} of Besov class $B_{\infty 1}^1(\mathbb{R})$, then trace formula (1.1) holds. The definition of the above Besov classes will be given in §2. Note that though these sufficient conditions are not necessary, the gap between the necessary conditions and the sufficient conditions obtained in [Pe1] and [Pe2] is rather narrow. Note also that in [ABF] a better sufficient condition was found; however, it seems to me that the condition $\varphi \in B_{\infty 1}^1$ is easier to work with.

In Koplienko's paper [Ko1] the author considered the case of perturbations of Hilbert-Schmidt class \mathcal{S}_2 . Let A and B be a self-adjoint operators such that $K \stackrel{\text{def}}{=} B - A \in \mathcal{S}_2$. In this case the operator $\varphi(B) - \varphi(A)$ does not have to be in \mathcal{S}_1 even for very nice functions φ . The idea of Koplienko was to consider the operator

$$\varphi(B) - \varphi(A) - \frac{d}{ds} \left(\varphi(A + sK) \right) \Big|_{s=0}$$

and find a trace formula under certain assumptions on φ . It was shown in [Ko1] that there exists a unique function $\eta \in L^1(\mathbb{R})$ such that

$$\text{trace} \left(\varphi(B) - \varphi(A) - \frac{d}{ds} \left(\varphi(A + sK) \right) \Big|_{s=0} \right) = \int_{\mathbb{R}} \varphi''(x) \eta(x) dx \quad (1.3)$$

for rational functions φ with poles off \mathbb{R} . The function η is called the *generalized spectral shift function corresponding to the pair (A, B)* .

A similar problem for unitary operators was considered by Neidhardt in [N]. Let U and V be unitary operators such that $V - U \in \mathcal{S}_2$. Then $V = \exp(iA)U$, where A is a self-adjoint operator in \mathcal{S}_2 . Put $U_s = e^{isA}U$, $s \in \mathbb{R}$. It was shown in [N] that there exists a function $\eta \in L^1(\mathbb{T})$ such that

$$\text{trace} \left(\varphi(V) - \varphi(U) - \frac{d}{ds} \left(\varphi(U_s) \right) \Big|_{s=0} \right) = \int_{\mathbb{T}} \varphi'' \eta dm, \quad (1.4)$$

whenever φ'' has absolutely convergent Fourier series. Such a function η is unique modulo a constant and it is called a *generalized spectral shift function corresponding to the pair* (U, V) .

We refer the reader to [Ko2] and [Bo] for applications of Koplienko's trace formula [Ko1].

In this paper we obtain better sufficient conditions on functions φ , under which trace formulae (1.3) and (1.4) hold. We consider the case of unitary operators in §3 and the case of self-adjoint operators in §4. We show that formula (1.3) holds under the assumption that φ belongs to the Besov class $B_{\infty 1}^2(\mathbb{R})$ while trace formula (1.4) holds whenever $\varphi \in B_{\infty 1}^2$. Note however, that the case of self-adjoint operators is considerably more complicated. First of all, unlike in the case of functions on \mathbb{T} the set of rational functions with poles off \mathbb{R} is not dense in $B_{\infty 1}^2(\mathbb{R})$. Second, functions in $\varphi \in B_{\infty 1}^2(\mathbb{R})$ do not have to be Lipschitz and it is not clear how to interpret each of the operators

$$\varphi(B) - \varphi(A) \quad \text{and} \quad \left. \frac{d}{ds} \left(\varphi(A + sK) \right) \right|_{s=0}.$$

However, it is still possible to define their difference and show that the difference belongs to \mathcal{S}_1 .

In §2 we outline the theory of double operator integrals developed by Birman and Solomyak in [BS1], [BS2], and [BS4], and we define Besov classes and discuss their properties.

2. Preliminaries

In this section we collect necessary information on double operator integrals and Besov classes.

Double operator integrals. The technique of double operator integrals developed by Birman and Solomyak in [BS1], [BS2], and [BS4] plays an important role in perturbation theory. We give here a brief introduction in this theory and state several results that will be used in the main part of this paper.

Let (\mathcal{X}, E) and (\mathcal{Y}, F) be spaces with spectral measures E and F on a Hilbert space \mathcal{H} . Double operator integrals are objects of the form

$$\int_{\mathcal{X}} \int_{\mathcal{Y}} \psi(x, y) dE(x) T dF(y), \tag{2.1}$$

where T is an operator on \mathcal{H} . Certainly, one has to specify how to understand the expression in (2.1). Let us first define double operator integrals for bounded functions ψ and operators T of Hilbert Schmidt class \mathcal{S}_2 . Consider the spectral measure \mathcal{E} whose values are orthogonal projections on the Hilbert space \mathcal{S}_2 , which is defined by

$$\mathcal{E}(\Delta \times \Lambda) T = E(\Delta) T F(\Lambda), \quad T \in \mathcal{S}_2,$$

for Δ and Λ being measurable subsets of \mathcal{X} and \mathcal{Y} . Then \mathcal{E} extends to a spectral measure on $\mathcal{X} \times \mathcal{Y}$ and if ψ is a bounded measurable function on $\mathcal{X} \times \mathcal{Y}$, by definition

$$\int_{\mathcal{X}} \int_{\mathcal{Y}} \psi(x, y) dE(x)T dF(y) = \left(\int_{\mathcal{X} \times \mathcal{Y}} \psi d\mathcal{E} \right) T.$$

Clearly,

$$\left\| \int_{\mathcal{X}} \int_{\mathcal{Y}} \psi(x, y) dE(x)T dF(y) \right\|_{\mathbf{S}_2} \leq \|\psi\|_{L^\infty} \|T\|_{\mathbf{S}_2}.$$

If

$$\int_{\mathcal{X}} \int_{\mathcal{Y}} \psi(x, y) dE(x)T dF(y) \in \mathbf{S}_1$$

for every $T \in \mathbf{S}_1$, we say that ψ is a *Schur multiplier* of \mathbf{S}_1 . In this case by duality the map

$$T \mapsto \int_{\mathcal{X}} \int_{\mathcal{Y}} \psi(x, y) dE(x)T dF(y)$$

extends to a bounded transformer on the space of bounded linear operators on \mathcal{H} .

Suppose now that A is a self-adjoint operator on a Hilbert space \mathcal{H} and $B = A + K$, where K is a self-adjoint operator of class \mathbf{S}_2 , and let φ be a Lipschitz function on \mathbb{R} , then $\varphi(B) - \varphi(A) \in \mathbf{S}_2$ and

$$\varphi(B) - \varphi(A) = \iint_{\mathbb{R} \times \mathbb{R}} \frac{\varphi(x) - \varphi(y)}{x - y} dE_B(x)K dE_A(y), \quad (2.2)$$

where E_A and E_B are spectral measure of A and B . Here we can define the function $(\varphi(x) - \varphi(y))(x - y)^{-1}$ on the diagonal $\{(x, x) : x \in \mathbb{R}\}$ in an arbitrary way.

A similar formula holds for unitary operators U and V with $V - U \in \mathbf{S}_2$:

$$\varphi(V) - \varphi(U) = \iint_{\mathbb{T} \times \mathbb{T}} \frac{\varphi(\zeta) - \varphi(\tau)}{\zeta - \tau} dE_V(\zeta)(V - U) dE_U(\tau), \quad (2.3)$$

where φ is a Lipschitz function on \mathbb{T} . Again, the right-hand side of this formula does not depend on the values of the function $(\varphi(\zeta) - \varphi(\tau))(\zeta - \tau)^{-1}$ on the diagonal $\{(\zeta, \zeta) : \zeta \in \mathbb{T}\}$. We refer the reader to [BS1], [BS2], and [BS4] for more detailed information on double operator integrals. We also mention recent survey article [BS5].

It follows from the results of [F] and [Pe1], [Pe2] mentioned in the introduction, that the conditions $\varphi \in C^1$ and $\varphi' \in L^\infty$ do not imply that the above double operator integrals determine bounded linear operators on \mathbf{S}_1 . On the other hand, it follows from the results of [Pe1] and [Pe2], that for functions φ in the Besov class $B_{\infty 1}^1$ on the circle and for functions φ in the Besov class $B_{\infty 1}^1(\mathbb{R})$ on \mathbb{R} the following estimates hold:

$$\left\| \iint_{\mathbb{T} \times \mathbb{T}} \frac{\varphi(\zeta) - \varphi(\tau)}{\zeta - \tau} dE_V(\zeta)(V - U) dE_U(\tau) \right\|_{\mathbf{S}_1} \leq \text{const} \|\varphi\|_{B_{\infty 1}^1} \|V - U\|_{\mathbf{S}_1} \quad (2.4)$$

and

$$\left\| \iint_{\mathbb{R} \times \mathbb{R}} \frac{\varphi(x) - \varphi(y)}{x - y} dE_B(x) K dE_A(y) \right\|_{\mathcal{S}_1} \leq \text{const} \|\varphi\|_{B_{\infty 1}^1(\mathbb{R})} \|K\|_{\mathcal{S}_1}.$$

In their papers [BS1], [BS2], and [BS4] Birman and Solomyak studied the problem of the differentiability of the map $t \mapsto \varphi(A + sK)$ in the operator norm and obtained sufficient conditions (a similar problems was also studied there in the case of functions of unitary operators). Later their results were improved in [Pe1] and [Pe2].

In this paper we need only differentiability results in the norm of \mathcal{S}_2 . Let φ be a function in $C^1(\mathbb{R})$ such that $\varphi' \in L^\infty$. Suppose that A is a self-adjoint operator (not necessarily bounded) and K is a self-adjoint operator of class \mathcal{S}_2 . Then

$$\frac{d}{ds} \left(\varphi(A + sK) \right) \Big|_{s=0} = \iint_{\mathbb{R} \times \mathbb{R}} \frac{\varphi(x) - \varphi(y)}{x - y} dE_A(x) K dE_A(y) \quad (2.5)$$

(the derivative exists in the \mathcal{S}_2 norm). This follows from formula (2.2) and Proposition 3.2 of [dPS].

A similar result holds for functions of unitary operators. Let $\varphi \in C^1(\mathbb{T})$. Suppose that U is a unitary operator, A is a self-adjoint operator of class \mathcal{S}_2 . Then

$$\frac{d}{ds} \left(\varphi(e^{isA}U) \right) \Big|_{s=0} = i \iint_{\mathbb{T} \times \mathbb{T}} \tau \frac{\varphi(\zeta) - \varphi(\tau)}{\zeta - \tau} dE_U(\zeta) A dE_U(\tau). \quad (2.6)$$

The proof of this formula is much simpler than in the case of possibly unbounded self-adjoint operators.

Besov classes. Let $0 < p, q \leq \infty$ and $s \in \mathbb{R}$. The Besov class B_{pq}^s of functions (or distributions) on \mathbb{T} can be defined in the following way. Let v be a C^∞ function on \mathbb{R} such that

$$w \geq 0, \quad \text{supp } w \subset \left[\frac{1}{2}, 2 \right], \quad \text{and} \quad \sum_{n=-\infty}^{\infty} w(2^n x) = 1 \quad \text{for } x > 0. \quad (2.7)$$

Consider the trigonometric polynomials W_n , and $W_n^\#$ defined by

$$W_n(z) = \sum_{k \in \mathbb{Z}} v \left(\frac{k}{2^n} \right), \quad n \geq 1, \quad W_0(z) = \bar{z} + 1 + z, \quad \text{and} \quad W_n^\#(z) = \overline{W_n(z)}, \quad n \geq 0.$$

Then for each distribution φ on \mathbb{T}

$$\varphi = \sum_{n \geq 0} \varphi * W_n + \sum_{n \geq 1} \varphi * W_n^\#.$$

The Besov class B_{pq}^s consists of functions (in the case $s > 0$) or distributions φ on \mathbb{T} such that

$$\{ \|2^{ns} \varphi * W_n\|_{L^p} \}_{n \geq 0} \in \ell^q \quad \text{and} \quad \{ \|2^{ns} \varphi * W_n^\#\|_{L^p} \}_{n \geq 0} \in \ell^q$$

Besov classes admit many other descriptions. in particular, for $s > 0$ the space B_{pq}^s can be described in terms of moduli of continuity (or moduli of smoothness).

To define (homogeneous) Besov classes $B_{pq}^s(\mathbb{R})$ on the real line, we consider the same function w as in (2.7) and define the functions W_n and $W_n^\#$ on \mathbb{R} by

$$\mathcal{F}W_n(x) = w\left(\frac{x}{2^n}\right), \quad \mathcal{F}W_n^\#(x) = \mathcal{F}W_n(-x), \quad n \in \mathbb{Z},$$

where \mathcal{F} is the *Fourier transform*. The Besov class $B_{pq}^s(\mathbb{R})$ consists of distributions φ on \mathbb{R} such that

$$\{\|2^{ns}\varphi * W_n\|_{L^p}\}_{n \in \mathbb{Z}} \in \ell^q(\mathbb{Z}) \quad \text{and} \quad \{\|2^{ns}\varphi * W_n^\#\|_{L^p}\}_{n \in \mathbb{Z}} \in \ell^q(\mathbb{Z})$$

According to this definition, the space $B_{pq}^s(\mathbb{R})$ contains all polynomials. However, it is not necessary to include all polynomials.

In this paper we need only Besov spaces $B_{\infty 1}^1$ and $B_{\infty 1}^2$. In the case of functions on the real line it is convenient to restrict the degree of polynomials in $B_{\infty 1}^1(\mathbb{R})$ by 1 and in $B_{\infty 1}^2(\mathbb{R})$ by 2. It is also convenient to consider the following seminorms on $B_{\infty 1}^1(\mathbb{R})$ and in $B_{\infty 1}^2(\mathbb{R})$:

$$\|\varphi\|_{B_{\infty 1}^1(\mathbb{R})} = \sup_{x \in \mathbb{R}} |\varphi'(x)| + \sum_{n \in \mathbb{Z}} 2^n \|\varphi * W_n\|_{L^\infty} + \sum_{n \in \mathbb{Z}} 2^n \|\varphi * W_n^\#\|_{L^\infty}$$

and

$$\|\varphi\|_{B_{\infty 1}^2(\mathbb{R})} = \sup_{x \in \mathbb{R}} |\varphi''(x)| + \sum_{n \in \mathbb{Z}} 2^{2n} \|\varphi * W_n\|_{L^\infty} + \sum_{n \in \mathbb{Z}} 2^{2n} \|\varphi * W_n^\#\|_{L^\infty}.$$

The classes $B_{\infty 1}^1(\mathbb{R})$ and $B_{\infty 1}^2(\mathbb{R})$ can be described as classes of function on \mathbb{R} in the following way:

$$\varphi \in B_{\infty 1}^1(\mathbb{R}) \quad \iff \quad \sup_{t \in \mathbb{R}} |\varphi'(t)| + \int_{\mathbb{R}} \frac{\|\Delta_t^2 \varphi\|_{L^\infty}}{|t|^2} dt < \infty$$

and

$$\varphi \in B_{\infty 1}^2(\mathbb{R}) \quad \iff \quad \sup_{t \in \mathbb{R}} |\varphi''(t)| + \int_{\mathbb{R}} \frac{\|\Delta_t^3 \varphi\|_{L^\infty}}{|t|^3} dt < \infty,$$

where Δ_t is the difference operator defined by $(\Delta_t \varphi)(x) = \varphi(x+t) - \varphi(x)$.

It is interesting to note that the Besov class $B_{\infty 1}^2(\mathbb{R})$ also appears in a natural way in perturbation theory in [Pe3], where the following problem is studied: in which case

$$\varphi(T_f) - T_{\varphi \circ f} \in \mathbf{S}_1?$$

(T_g is a Toeplitz operator with symbol g .)

We refer the reader to [Pee] for more detailed information on Besov classes.

3. The case of unitary operators

Let U and V be unitary operators such that $V - U \in \mathbf{S}_2$. Denote by E_U and E_V the spectral measures of U and V . Let A be a self-adjoint operator such that $\sigma(A) \subset [-\pi, \pi]$ and $V = \exp(iA)U$. It is easy to see that $A \in \mathbf{S}_2$.

Put

$$U_s = e^{isA}U. \quad (3.1)$$

Consider the class $\text{Lip} \hat{\otimes} L^\infty$ that consists of functions u on $\mathbb{T} \times \mathbb{T}$ that admit a representation

$$u(\zeta, \tau) = \sum_{n \geq 0} f_n(\zeta) g_n(\tau), \quad \zeta, \tau \in \mathbb{T}, \quad (3.2)$$

where $f_n \in \text{Lip}$, $g_n \in L^\infty$, and

$$\sum_{n \geq 0} \|f_n\|_{\text{Lip}} \cdot \|g_n\|_\infty < \infty. \quad (3.3)$$

By definition, $\|u\|_{\text{Lip} \hat{\otimes} L^\infty}$ is the infimum of the left-hand side of (3.3) over all functions f_n and g_n satisfying (3.2). We consider here the following seminorm on the space Lip of Lipschitz functions:

$$\|f\|_{\text{Lip}} = \sup_{\zeta \neq \tau} \frac{|f(\zeta) - f(\tau)|}{|\zeta - \tau|}.$$

For a differentiable function φ on \mathbb{T} we define the function $\check{\varphi}$ on $\mathbb{T} \times \mathbb{T}$ by

$$\check{\varphi}(\zeta, \tau) = \begin{cases} \frac{\varphi(\zeta) - \varphi(\tau)}{\zeta - \tau}, & \zeta \neq \tau, \\ \varphi'(\zeta), & \zeta = \tau. \end{cases}$$

Theorem 3.1. *If $\varphi \in B_{\infty 1}^2$, then*

$$\varphi(V) - \varphi(U) - \frac{d}{ds} \left(\varphi(U_s) \right) \Big|_{s=0} \in \mathbf{S}_1 \quad (3.4)$$

and

$$\left\| \varphi(V) - \varphi(U) - \frac{d}{ds} \left(\varphi(U_s) \right) \Big|_{s=0} \right\|_{\mathbf{S}_1} \leq \text{const} \|\varphi\|_{B_{\infty 1}^2} \|V - U\|_{\mathbf{S}_2}.$$

To prove Theorem 3.1, we need the following fact.

Theorem 3.2. *If $\varphi \in B_{\infty 1}^2$, then $\check{\varphi} \in \text{Lip} \hat{\otimes} L^\infty$ and*

$$\|\check{\varphi}\|_{\text{Lip} \hat{\otimes} L^\infty} \leq \text{const} \|\varphi\|_{B_{\infty 1}^2}.$$

Proof. We have

$$\check{\varphi}(\zeta, \tau) = \sum_{j, k \geq 0} \hat{\varphi}(j+k+1) \zeta^j \tau^k + \sum_{j, k < 0} \hat{\varphi}(j+k+1) \zeta^j \tau^k. \quad (3.5)$$

Let us show that the first term on the right-hand side of (3.5) belongs to $\text{Lip} \hat{\otimes} L^\infty$. A similar result for the second term in (3.5) can be proved in the same way. We use the construction given in the proof of Theorem 2 of Section 3 of [Pe1]. We have

$$\sum_{j, k \geq 0} \hat{\varphi}(j+k+1) \zeta^j \tau^k = \sum_{j, k \geq 0} \alpha_{jk} \hat{\varphi}(j+k+1) \zeta^j \tau^k + \sum_{j, k \geq 0} \beta_{jk} \hat{\varphi}(j+k+1) \zeta^j \tau^k, \quad (3.6)$$

where

$$\alpha_{jk} = \begin{cases} \frac{1}{2}, & j = k = 0, \\ \frac{2j-k}{j+k}, & j+k > 0, \frac{k}{2} \leq j \leq 2k, \\ 0, & j \geq 2k, \end{cases} \quad \text{and} \quad \beta_{jk} = 1 - \alpha_{jk}.$$

Let us prove that the function

$$(\zeta, \tau) \mapsto \sum_{j,k \geq 0} \beta_{jk} \hat{\varphi}(j+k+1) \zeta^j \tau^k$$

on the right-hand side of (3.6) belongs to $\text{Lip} \hat{\otimes} L^\infty$.

We define the functions q and r on \mathbb{R} by

$$q(x) = \begin{cases} 0, & x \leq \frac{1}{2}, \\ \frac{2x-1}{x+1}, & \frac{1}{2} \leq x \leq 2, \\ 1, & x \geq 2, \end{cases} \quad \text{and} \quad r(x) = \begin{cases} 0, & x \leq \frac{3}{2}, \\ \frac{2x-3}{x}, & \frac{3}{2} \leq x \leq 3, \\ 1, & x \geq 3. \end{cases} \quad (3.7)$$

Put

$$Q_n(z) = \sum_{j \geq 0} q\left(\frac{j}{n}\right), \quad R_n(z) = \sum_{j \geq 0} r\left(\frac{j}{n}\right) \quad \text{for } n > 0$$

and

$$Q_0(z) = R_0(z) = \frac{1}{2} + \sum_{j \geq 1} z^j.$$

It is easy to see that

$$\sum_{j,k \geq 0} \beta_{jk} \hat{\varphi}(j+k+1) \zeta^j \tau^k = \sum_{n \geq 0} \zeta^n \left(((S^*)^n \psi * Q_n)(\tau) \right), \quad (3.8)$$

where $\psi = \mathbb{P}_+ \bar{z} \varphi$ and $S^* \psi = \frac{\psi - \psi(0)}{z}$. We have

$$\sum_{n \geq 0} \|z^n\|_{\text{Lip}} \| (S^*)^n \psi * Q_n \|_\infty \leq \text{const} \sum_{n \geq 0} n \| (S^*)^n \psi * Q_n \|_\infty = \text{const} \sum_{n \geq 0} n \| \psi * R_n \|_\infty.$$

Let us show that for $\varphi \in B_{\infty 1}^2$,

$$\sum_{n \geq 0} n \| \psi * R_n \|_\infty < \infty.$$

Consider the function r^\flat on \mathbb{R} defined by $r^\flat(x) = 1 - r(|x|)$, $x \in \mathbb{R}$. Put

$$R_n^\flat(z) = \sum_{j \in \mathbb{Z}} r^\flat\left(\frac{j}{n}\right), \quad n > 0.$$

then $\|R_n^\flat\|_{L^1} \leq \text{const}$ (see the proof of Lemma 3 of [Pe1]). Suppose that $n \geq 2^m$. Then

$$R_n * \psi = R_n * \sum_{k \geq m} \psi * W_k$$

(see §2 for the definition of the polynomials W_k). Hence,

$$\|R_n * \psi\|_\infty \leq \left\| R_n * \left(\sum_{k \geq m} \psi * W_k \right) \right\|_\infty \leq (1 + \|R_n^b\|_1) \sum_{k \geq m} \|\psi * W_k\|_\infty.$$

It follows that

$$\begin{aligned} \sum_{n \geq 2} n \|\psi * R_n\|_\infty &= \sum_{m \geq 1} \sum_{n=2^m}^{2^{m+1}-1} n \|\psi * R_n\|_\infty \\ &\leq \text{const} \sum_{m \geq 1} 2^{2m} \sum_{k \geq m} \|\psi * W_k\|_\infty \leq \text{const} \sum_{m \geq 1} 2^{2m} \|\psi * W_m\|_\infty < \infty, \end{aligned}$$

since $\psi \in B_{\infty 1}^2$.

Let us now show that the function

$$(\zeta, \tau) \mapsto \sum_{j, k \geq 0} \alpha_{jk} \hat{\varphi}(j+k+1) \zeta^j \tau^k$$

belongs to the space $\text{Lip} \hat{\otimes} L^\infty$.

It follows from (3.8) that

$$\sum_{j, k \geq 0} \alpha_{jk} \hat{\varphi}(j+k+1) \zeta^j \tau^k = \sum_{n \geq 0} \left(((S^*)^n \psi * Q_n)(\zeta) \right) \tau^n.$$

It suffices to show that

$$\sum_{n \geq 0} \|((S^*)^n \psi * Q_n)\|_{\text{Lip}} < \infty.$$

By the Bernstein inequality, we have

$$\begin{aligned} \sum_{n \geq 0} \|((S^*)^n \psi * Q_n)\|_{\text{Lip}} &= \sum_{n \geq 0} \left\| \left(((S^*)^n \psi * Q_n)' \right) \right\|_\infty \\ &\leq \sum_{n \geq 0} \sum_{k \geq 0} \left\| \left(((S^*)^n (\psi * W_k)) * Q_n \right)' \right\|_\infty \\ &\leq \sum_{n \geq 0} \sum_{k \geq 0} 2^{k+1} \|((S^*)^n (\psi * W_k)) * Q_n\|_\infty \\ &\leq \sum_{n \geq 0} \sum_{k \geq 0} 2^{k+1} \|\psi * W_k * R_n\|_\infty \\ &\leq \sum_{0 \leq n \leq 2^{k+2}/3} (1 + \|R_n^b\|_1) \sum_{k \geq 0} 2^{k+1} \|\psi * W_k\|_\infty \\ &\leq \text{const} \sum_{k \geq 0} 2^{2k} \|\psi * W_k\|_\infty \leq \text{const} \|\psi\|_{B_{\infty 1}^2}, \end{aligned}$$

since, clearly, $\psi * W_k * R_n = \mathbf{0}$ if $n > 2^{k+2}/3$. ■

Proof of Theorem 3.1. Since $\varphi \in C^1(\mathbb{T})$, we have by (2.6)

$$\frac{d}{ds} \left(\varphi(U_s) \right) \Big|_{s=0} = \mathbf{i} \iint_{\mathbb{T} \times \mathbb{T}} \tau \check{\varphi}(\zeta, \tau) dE_U(\zeta) A dE_U(\tau).$$

On the other hand, by (2.3),

$$\begin{aligned} \varphi(V) - \varphi(U) &= \iint_{\mathbb{T} \times \mathbb{T}} \check{\varphi}(\zeta, \tau) dE_V(\zeta) (V - U) dE_U(\tau) \\ &= - \iint_{\mathbb{T} \times \mathbb{T}} \tau \check{\varphi}(\zeta, \tau) dE_V(\zeta) (I - VU^*) dE_U(\tau) \\ &= - \iint_{\mathbb{T} \times \mathbb{T}} \tau \check{\varphi}(\zeta, \tau) dE_V(\zeta) (I - e^{\mathbf{i}A}) dE_U(\tau). \end{aligned}$$

Thus

$$\begin{aligned} \varphi(V) - \varphi(U) - \frac{d}{ds} \left(\varphi(U_s) \right) \Big|_{s=0} &= - \iint_{\mathbb{T} \times \mathbb{T}} \tau \check{\varphi}(\zeta, \tau) dE_V(\zeta) (I - e^{\mathbf{i}A}) dE_U(\tau) \\ &\quad - \mathbf{i} \iint_{\mathbb{T} \times \mathbb{T}} \tau \check{\varphi}(\zeta, \tau) dE_U(\zeta) A dE_U(\tau) \\ &= - \iint_{\mathbb{T} \times \mathbb{T}} \tau \check{\varphi}(\zeta, \tau) dE_V(\zeta) (I - e^{\mathbf{i}A}) dE_U(\tau) \\ &\quad + \iint_{\mathbb{T} \times \mathbb{T}} \tau \check{\varphi}(\zeta, \tau) dE_U(\zeta) (I - e^{\mathbf{i}A}) dE_U(\tau) \\ &\quad + \iint_{\mathbb{T} \times \mathbb{T}} \tau \check{\varphi}(\zeta, \tau) dE_U(\zeta) (e^{\mathbf{i}A} - I - \mathbf{i}A) dE_U(\tau). \end{aligned}$$

It is easy to see that $e^{\mathbf{i}A} - I - \mathbf{i}A \in \mathbf{S}_1$, and so by (2.4),

$$\iint_{\mathbb{T} \times \mathbb{T}} \tau \check{\varphi}(\zeta, \tau) dE_U(\zeta) (e^{\mathbf{i}A} - I - \mathbf{i}A) dE_U(\tau) \in \mathbf{S}_1$$

and

$$\left\| \iint_{\mathbb{T} \times \mathbb{T}} \tau \check{\varphi}(\zeta, \tau) dE_U(\zeta) (e^{\mathbf{i}A} - I - \mathbf{i}A) dE_U(\tau) \right\|_{\mathbf{S}_1} \leq \text{const} \|\varphi\|_{B_{\infty 1}^1} \| (e^{\mathbf{i}A} - I - \mathbf{i}A) \|_{\mathbf{S}_1}.$$

Clearly, $\|\varphi\|_{B_{\infty 1}^1} \leq \text{const} \|\varphi\|_{B_{\infty 1}^2}$.

On the other hand, let $\{f_n\}_{n \geq 0}$ and $\{g_n\}_{n \geq 0}$ be sequences of functions such that

$$\check{\varphi}(\zeta, \tau) = \sum_{n \geq 0} f_n(\zeta) g_n(\tau), \quad \zeta, \tau \in \mathbb{T},$$

and (3.3) holds. We have

$$\begin{aligned} & \iint_{\mathbb{T} \times \mathbb{T}} \tau \check{\varphi}(\zeta, \tau) dE_V(\zeta) (I - e^{iA}) dE_U(\tau) - \iint_{\mathbb{T} \times \mathbb{T}} \tau \check{\varphi}(\zeta, \tau) dE_U(\zeta) (I - e^{iA}) dE_U(\tau) \\ &= \iint_{\mathbb{T} \times \mathbb{T}} \sum_{n \geq 0} f_n(\zeta) \tau g_n(\tau) dE_V(\zeta) (I - e^{iA}) dE_U(\tau) \\ & \quad - \iint_{\mathbb{T} \times \mathbb{T}} \sum_{n \geq 0} f_n(\zeta) \tau g_n(\tau) dE_U(\zeta) (I - e^{iA}) dE_U(\tau) \\ &= \sum_{n \geq 0} f_n(V) (I - e^{iA}) g_n(U) U - \sum_{n \geq 0} f_n(U) (I - e^{iA}) g_n(U) U \\ &= \sum_{n \geq 0} (f_n(V) - f_n(U)) (I - e^{iA}) g_n(U) U. \end{aligned}$$

Thus

$$\begin{aligned} & \left\| \iint_{\mathbb{T} \times \mathbb{T}} \tau \check{\varphi}(\zeta, \tau) dE_V(\zeta) (I - e^{iA}) dE_U(\tau) - \iint_{\mathbb{T} \times \mathbb{T}} \tau \check{\varphi}(\zeta, \tau) dE_U(\zeta) (I - e^{iA}) dE_U(\tau) \right\|_{\mathbf{S}_1} \\ & \leq \sum_{n \geq 0} \| (f_n(V) - f_n(U)) \|_{\mathbf{S}_2} \| (I - e^{iA}) \|_{\mathbf{S}_2} \| g_n(U) \| \\ & \leq \text{const} \| (I - e^{iA}) \|_{\mathbf{S}_2} \sum_{n \geq 0} \| f_n \|_{\text{Lip}} \cdot \| g_n \|_{\infty} < \infty. \end{aligned}$$

This completes the proof. \blacksquare

Let now η be a generalized spectral shift function for the pair (V, U) .

Theorem 3.3. *Let U and V be unitary operators such that $V - U \in \mathbf{S}_2$ and let U_s be defined by (4.1). Then for any $\varphi \in B_{\infty 1}^2$,*

$$\text{trace} \left(\varphi(V) - \varphi(U) - \frac{d}{ds} \left(\varphi(U_s) \right) \Big|_{s=0} \right) = \int_{\mathbb{T}} \varphi'' \eta d\mathbf{m}. \quad (3.9)$$

Proof. Since clearly, $B_{\infty 1}^2 \subset C^1$, the fact that the operator in (3.4) belongs to \mathbf{S}_1 is an immediate consequence of Theorems 3.1 and 3.2.

It is easy to see from the definition of the space $B_{\infty 1}^2$ given in §2 that the trigonometric polynomials are dense in $B_{\infty 1}^2$. Let φ_n be trigonometric polynomials such that

$$\lim_{n \rightarrow \infty} \|\varphi - \varphi_n\|_{B_{\infty 1}^2} = 0.$$

Since $B_{\infty 1}^2$ is continuously imbedded in the space C^2 of functions with two continuous derivatives, it follows that $\varphi_n \rightarrow \varphi$ in C^2 . Since $\eta \in L^1$, it follows that

$$\lim_{n \rightarrow \infty} \int_{\mathbb{T}} \varphi_n'' \eta \, d\mathbf{m} = \int_{\mathbb{T}} \varphi'' \eta \, d\mathbf{m}.$$

On the other hand, it follows from Theorems 3.1 and 3.2 that

$$\left\| \left(\varphi_n(V) - \varphi_n(U) - \frac{d}{ds} \left(\varphi_n(U_s) \right) \Big|_{s=0} \right) - \left(\varphi(V) - \varphi(U) - \frac{d}{ds} \left(\varphi(U_s) \right) \Big|_{s=0} \right) \right\|_{\mathcal{S}_1} \rightarrow 0$$

as $n \rightarrow \infty$. The result follows now from the fact that trace formula (3.9) is valid for all trigonometric polynomials φ (see [N]). ■

4. The case of self-adjoint operators

In this section we extend Koplienko's trace formula for self-adjoint operators to a considerably bigger class of functions.

Let A be a self-adjoint operator (not necessarily bounded) on Hilbert space and let K be a self-adjoint operator of class \mathcal{S}_2 . Put $B = A + K$. As we have already mentioned in the introduction, Koplienko introduced in [Ko1] the generalized spectral shift function $\eta \in L^1$ that corresponds to the pair (A, B) and showed that for rational functions φ with poles off the real line the following trace formula holds.

$$\text{trace} \left(\varphi(B) - \varphi(A) - \frac{d}{ds} \left(\varphi(A_s) \right) \Big|_{s=0} \right) = \int_{\mathbb{R}} \varphi''(x) \eta(x) \, dx. \quad (4.1)$$

We are going to extend this formula to the Besov class $B_{\infty 1}^2(\mathbb{R})$. Note however, that the situation with self-adjoint operators is subtler than with unitary operators. First of all, the rational functions are not dense in $B_{\infty 1}^2(\mathbb{R})$ and this makes it more difficult to extend formula (4.1) from rational functions to $B_{\infty 1}^2(\mathbb{R})$. Secondly, functions in $B_{\infty 1}^2(\mathbb{R})$ do not have to belong to the space Lip of Lipschitz functions on \mathbb{R} , which we equip with the seminorm:

$$\|f\|_{\text{Lip}} = \sup_{x \neq y} \frac{|f(x) - f(y)|}{|x - y|}.$$

Thus for $\varphi \in B_{\infty 1}^2(\mathbb{R})$, none of the operators

$$\varphi(B) - \varphi(A) \quad \text{and} \quad \frac{d}{ds} \left(\varphi(A_s) \right) \Big|_{s=0}$$

has to be in \mathcal{S}_2 . In fact, it is not clear how one can interpret each of those operators. However, it turns out that their difference still makes sense for functions $\varphi \in B_{\infty 1}^2(\mathbb{R})$ and formula (4.1) holds for such functions φ .

To do it, we first prove formula (4.1) in the case $\varphi \in B_{\infty 1}^2(\mathbb{R}) \cap \text{Lip}$ and estimate the \mathcal{S}_1 norm of the left-hand side of (4.1) in terms of $\|\varphi\|_{B_{\infty 1}^2}$. Then we define the operator on the left-hand side of (4.1) for functions $f \in B_{\infty 1}^2(\mathbb{R})$ and prove formula (4.1) for such functions.

For a differentiable function φ on \mathbb{R} we define the function $\check{\varphi}$ on $\mathbb{R} \times \mathbb{R}$ by

$$\check{\varphi}(x, y) = \begin{cases} \frac{\varphi(x) - \varphi(y)}{\zeta^{-\tau}}, & x \neq y, \\ \varphi'(x), & x = y. \end{cases}$$

We consider in this section the space $\text{Lip} \hat{\otimes}_i L^\infty$ of functions u on $\mathbb{R} \times \mathbb{R}$ that admit a representation

$$u(x, y) = \int_{\Omega} f_{\omega}(x) g_{\omega}(y) d\mu(\omega), \quad (4.2)$$

where (Ω, μ) is a measure space and the functions $(\omega, x) \mapsto f_{\omega}(x)$ and $(\omega, y) \mapsto g_{\omega}(y)$ are measurable functions on $\Omega \times \mathbb{R}$ such that $f_{\omega} \in \text{Lip}$, $g_{\omega} \in L^\infty$ for almost all $\omega \in \Omega$, and

$$\int_{\Omega} \|f_{\omega}\|_{\text{Lip}} \cdot \|g_{\omega}\|_{L^\infty} d\mu(\omega) < \infty. \quad (4.3)$$

By definition, the norm of u in $\text{Lip} \hat{\otimes}_i L^\infty$ is the infimum of the left-hand side of (4.3) over all representations of the form (4.2).

Theorem 4.1. *Let $M > 0$. Suppose that φ is a bounded function on \mathbb{R} such that $\text{supp } \mathcal{F}\varphi \subset [M/2, 2M]$. Then*

$$\varphi(B) - \varphi(A) - \left. \frac{d}{ds} (\varphi(A_s)) \right|_{s=0} \in \mathbf{S}_1 \quad (4.4)$$

and

$$\left\| \varphi(B) - \varphi(A) - \left. \left(\frac{d}{ds} \varphi(A_s) \right) \right|_{s=0} \right\|_{\mathbf{S}_1} \leq \text{const} \cdot M^2 \|K\|_{\mathbf{S}_2}^2 \|\varphi\|_{L^\infty}. \quad (4.5)$$

To prove Theorem 4.1, we need the following fact.

Lemma 4.2. *Let φ be a function on \mathbb{R} such that $\text{supp } \mathcal{F}\varphi \subset [M/2, 2M]$. Then $\check{\varphi} \in \text{Lip} \hat{\otimes}_i L^\infty$ and*

$$\|\check{\varphi}\|_{\text{Lip} \hat{\otimes}_i L^\infty} \leq \text{const} \cdot M^2 \|\varphi\|_{L^\infty}.$$

Proof. Let q and r be the functions on \mathbb{R} defined by (3.7).

Consider the distributions Q_t and R_t , $t > 0$, on \mathbb{R} such that

$$(\mathcal{F}Q_t)(x) = q(x/t) \quad \text{and} \quad (\mathcal{F}R_t)(x) = r(x/t).$$

It was shown in [Pe2] (formula (5)) that

$$\check{\varphi}(x, y) = \int_0^\infty \left((S_t^* \varphi) * Q_t \right)(x) e^{ity} dt + \int_0^\infty \left((S_t^* \varphi) * Q_t \right)(y) e^{itx} dt, \quad (4.6)$$

where $(S_t^* \varphi)(x) = e^{-itx} \varphi(x)$.

Clearly,

$$\|\check{\varphi}\|_{\text{Lip} \hat{\otimes}_i L^\infty} \leq \int_0^\infty \|(S_t^* \varphi) * Q_t\|_{\text{Lip}} dt + \int_0^\infty \|(S_t^* \varphi) * Q_t\|_{L^\infty} t dt.$$

By the Bernstein inequality,

$$\|(S_t^* \varphi) * Q_t\|_{\text{Lip}} = \left\| \left((S_t^* \varphi) * Q_t \right)' \right\|_{L^\infty} \leq 2M \|(S_t^* \varphi) * Q_t\|_{L^\infty},$$

and so

$$\begin{aligned} \int_0^\infty \|(S_t^* \varphi) * Q_t\|_{\text{Lip}} dt &\leq 2M \int_0^\infty \|(S_t^* \varphi) * Q_t\|_{L^\infty} dt = 2M \int_0^\infty \|\varphi * R_t\|_{L^\infty} dt \\ &= 2M \int_0^{4M/3} \|\varphi * R_t\|_{L^\infty} dt \leq \frac{8}{3} M^2 \|\varphi * R_t\|_{L^\infty}, \end{aligned}$$

since, obviously, $(S_t^* \varphi) * R_t = \mathbf{0}$ for $t \geq 4M/3$.

On the other hand,

$$\begin{aligned} \int_0^\infty \|(S_t^* \varphi) * Q_t\|_{L^\infty} t dt &= \int_0^\infty \|\varphi * R_t\|_{L^\infty} t dt \\ &= \int_0^{4M/3} \|\varphi * R_t\|_{L^\infty} t dt. \end{aligned}$$

It remains to observe that if R_t^b is the function on \mathbb{R} such that

$$\mathcal{F}(R_t^b)(x) = 1 - \mathcal{F}(R_t)(|x|),$$

then $R_t^b \in L^1$, $\|R_t^b\|_{L^1}$ does not depend on t and

$$\|\varphi * R_t\|_{L^\infty} \leq (1 + \|R_t^b\|_{L^1}) \|\varphi\|_{L^\infty}. \quad \blacksquare$$

Proof of Theorem 4.1. By (2.2) and (2.5), we have

$$\begin{aligned} \varphi(B) - \varphi(A) - \frac{d}{ds}(\varphi(A_s)) \Big|_{s=0} &= \iint_{\mathbb{R} \times \mathbb{R}} \check{\varphi}(x, y) dE_B(x) K dE_A(y) \\ &\quad - \iint_{\mathbb{R} \times \mathbb{R}} \check{\varphi}(x, y) dE_A(x) K dE_A(y). \end{aligned} \quad (4.7)$$

By Lemma 4.2, $\check{\varphi}$ admits a representation

$$\check{\varphi}(x, y) = \int_{\Omega} f_\omega(x) g_\omega(y) d\mu(\omega)$$

such that

$$\int_{\Omega} \|f_\omega\|_{\text{Lip}} \cdot \|g_\omega\|_{L^\infty} d\mu(\omega) \leq \text{const} \cdot M^2 \|\varphi\|_{L^\infty}.$$

We have

$$\begin{aligned} \iint_{\mathbb{R} \times \mathbb{R}} \check{\varphi}(x, y) dE_B(x) K dE_A(y) &= \int_{\Omega} \left(\iint_{\mathbb{R} \times \mathbb{R}} f_\omega(x) g_\omega(y) dE_B(x) K dE_A(y) \right) d\mu(\omega) \\ &= \int_{\Omega} f_\omega(B) K g_\omega(A) d\mu(\omega). \end{aligned}$$

Similarly,

$$\iint_{\mathbb{R} \times \mathbb{R}} \check{\varphi}(x, y) dE_A(x) K dE_A(y) = \int_{\Omega} f_{\omega}(A) K g_{\omega}(A) d\mu(\omega).$$

Thus

$$\varphi(B) - \varphi(A) - \frac{d}{ds} \left(\varphi(A + sK) \right) \Big|_{s=0} = \int_{\Omega} (f_{\omega}(B) - f_{\omega}(A)) K g_{\omega}(A) d\mu(\omega).$$

Hence,

$$\begin{aligned} \left\| \varphi(B) - \varphi(A) - \frac{d}{ds} \left(\varphi(A_s) \right) \Big|_{s=0} \right\|_{\mathcal{S}_1} &\leq \int_{\Omega} \|f_{\omega}(B) - f_{\omega}(A)\|_{\mathcal{S}_2} \|K\|_{\mathcal{S}_2} \|g_{\omega}(A)\| d\mu(\omega) \\ &\leq \|K\|_{\mathcal{S}_2} \int_{\Omega} \|f_{\omega}\|_{\text{Lip}} \|B - A\|_{\mathcal{S}_2} \|g_{\omega}\|_{L^{\infty}} d\mu(\omega) \\ &= \|K\|_{\mathcal{S}_2}^2 \int_{\Omega} \|f_{\omega}\|_{\text{Lip}} \|g_{\omega}\|_{L^{\infty}} d\mu(\omega) \\ &\leq \text{const} \cdot M^2 \|K\|_{\mathcal{S}_2}^2 \|\varphi\|_{L^{\infty}}. \quad \blacksquare \end{aligned}$$

Remark. It is easy to see that the same conclusion holds if φ is a bounded function on \mathbb{R} such that $\text{supp } \mathcal{F}\varphi \subset [-2M, -M/2]$.

Theorem 4.3. *Suppose that $\varphi \in B_{\infty 1}^2(\mathbb{R}) \cap \text{Lip}$. Then (4.4) holds,*

$$\left\| \varphi(B) - \varphi(A) - \frac{d}{ds} \left(\varphi(A_s) \right) \Big|_{s=0} \right\|_{\mathcal{S}_1} \leq \text{const} \cdot \|K\|_{\mathcal{S}_2}^2 \|\varphi\|_{B_{\infty 1}^2},$$

and (4.1) holds.

We need the following lemma.

Lemma 4.4. *Let $\{f_n\}_{n \geq 0}$ and f be functions in $\text{Lip}(\mathbb{R})$ such that*

$$\lim_{n \rightarrow \infty} f_n(x) = f(x), \quad x \in \mathbb{R}, \quad \text{and} \quad \sup_n \|f_n\|_{\text{Lip}} < \infty.$$

Then

$$\lim_{n \rightarrow \infty} (f_n(B) - f_n(A)) = f(B) - f(A)$$

in \mathcal{S}_2 .

Let us first prove Theorem 4.3.

Proof of Theorem (4.3). Since $\varphi \in B_{\infty 1}^2(\mathbb{R})$, φ is continuously differentiable, and so both operators

$$\varphi(B) - \varphi(A) \quad \text{and} \quad \frac{d}{ds} \left(\varphi(A + sK) \right) \Big|_{s=0}$$

belong to \mathcal{S}_2 (see §2).

Clearly, if φ is a linear function, then the operator in (4.4) is zero. Suppose first that $\mathcal{F}\varphi'' \in L^1$. Then

$$\varphi = \sum_{n \in \mathbb{Z}} (\varphi_n + \varphi_n^\#).$$

where

$$\varphi_n = \varphi * \mathcal{F}^{-1} \chi_{[2^n, 2^{n+1}]} \quad \text{and} \quad \varphi_n^\# = \varphi * \mathcal{F}^{-1} \chi_{[-2^{n+1}, -2^n]}.$$

Clearly,

$$2^{2n} \|\varphi_n\|_{L^\infty} \leq \text{const} \|\mathcal{F}\varphi_n''\|_{L^1} \quad \text{and} \quad 2^{2n} \|\varphi_n^\#\|_{L^\infty} \leq \text{const} \|\mathcal{F}\varphi_n^\#\|_{L^1}. \quad (4.8)$$

By Theorem 4.1,

$$\sum_{n \in \mathbb{Z}} \left\| \varphi_n(B) - \varphi_n(A) - \frac{d}{ds} (\varphi_n(A_s)) \Big|_{s=0} \right\|_{\mathcal{S}_1} \leq \text{const} \sum_{n \in \mathbb{Z}} 2^{2n} \|\varphi_n\|_{L^\infty}$$

and the same estimate holds for the functions $\varphi_n^\#$ in place of φ_n . It follows now from (4.8) that

$$\begin{aligned} \left\| \varphi(B) - \varphi(A) - \frac{d}{ds} (\varphi(A_s)) \Big|_{s=0} \right\|_{\mathcal{S}_1} &\leq \text{const} \sum_{n \in \mathbb{Z}} 2^{2n} (\|\varphi_n\|_{L^\infty} + \|\varphi_n^\#\|_{L^\infty}) \\ &\leq \text{const} \|\mathcal{F}\varphi''\|_{L^1}. \end{aligned}$$

Since the rational functions are dense in the space $\{\varphi : \mathcal{F}\varphi'' \in L^1\}$ and trace formula (4.1) holds for rational functions with poles outside \mathbb{R} (Koplienko's theorem [Ko1]), it is easy to see that it also holds for arbitrary functions φ with $\mathcal{F}\varphi'' \in L^1$.

Suppose now that $\varphi \in B_{\infty 1}^2$. Since

$$\sum_{n \in \mathbb{Z}} 2^{2n} (\|\varphi * W_n\|_{L^\infty} + \|\varphi * W_n^\#\|_{L^\infty}) < \infty,$$

and inequality (4.5) holds, it suffices to show that formula (4.1) holds for functions $\varphi * W_n$ and $\varphi * W_n^\#$.

The following argument is similar to the argument given in the proof of Theorem 4 of [Pe2] to establish the Lifshitz–Krein trace formula for functions in $B_{\infty 1}^1(\mathbb{R})$. Put $\psi = \varphi * V_n$. Then $\text{supp } \psi \subset [2^{n-1}, 2^{n+1}]$. Consider a smooth nonnegative function h on \mathbb{R} such that $\text{supp } h \subset [-1, 1]$ and $\int_{-1}^1 h(x) dx = 1$. For $\varepsilon > 0$ put $h_\varepsilon(x) = \varepsilon^{-1} h(x/\varepsilon)$. Let ψ_ε be the function defined by $\mathcal{F}\psi_\varepsilon = \mathcal{F}\psi * h_\varepsilon$. Clearly,

$$\mathcal{F}\psi_\varepsilon \in L^1, \quad \lim_{\varepsilon \rightarrow 0} \|\psi_\varepsilon\|_{L^\infty} = \|\psi\|_{L^\infty}, \quad \text{and} \quad \lim_{\varepsilon \rightarrow 0} \psi_\varepsilon(x) = \psi(x) \quad \text{for } x \in \mathbb{R}.$$

Then formula (4.1) holds for ψ_ε . Clearly,

$$\lim_{\varepsilon \rightarrow 0} \int_{\mathbb{R}} \psi_\varepsilon''(x) \eta(x) dx = \int_{\mathbb{R}} \psi''(x) \eta(x) dx.$$

Thus to prove that (4.1) holds for ψ , it suffices to show that

$$\lim_{\varepsilon \rightarrow 0} \text{trace} \left(\psi_\varepsilon(B) - \psi_\varepsilon(A) - \frac{d}{ds} (\psi_\varepsilon(A_s)) \Big|_{s=0} \right) = \text{trace} \left(\psi(B) - \psi(A) - \frac{d}{ds} (\psi(A_s)) \Big|_{s=0} \right).$$

By (4.7), we have

$$\begin{aligned} \psi_\varepsilon(B) - \psi_\varepsilon(A) - \frac{d}{ds} \left(\psi_\varepsilon(A_s) \right) \Big|_{s=0} &= \iint_{\mathbb{R} \times \mathbb{R}} \check{\psi}_\varepsilon(x, y) dE_B(x) K dE_A(y) \\ &\quad - \iint_{\mathbb{R} \times \mathbb{R}} \check{\psi}_\varepsilon(x, y) dE_A(x) K dE_A(y). \end{aligned}$$

By (4.6), this is equal to

$$\begin{aligned} &\int_0^\infty \iint_{\mathbb{R} \times \mathbb{R}} \left((S_t^* \psi_\varepsilon) * Q_t \right) (x) e^{ity} dE_B(x) K dE_A(y) dt + \\ &\int_0^\infty \iint_{\mathbb{R} \times \mathbb{R}} \left((S_t^* \psi_\varepsilon) * Q_t \right) (y) e^{itx} dE_B(x) K dE_A(y) dt - \\ &\int_0^\infty \iint_{\mathbb{R} \times \mathbb{R}} \left((S_t^* \psi_\varepsilon) * Q_t \right) (x) e^{ity} dE_A(x) K dE_A(y) dt - \\ &\int_0^\infty \iint_{\mathbb{R} \times \mathbb{R}} \left((S_t^* \psi_\varepsilon) * Q_t \right) (y) e^{itx} dE_A(x) K dE_A(y) dt. \end{aligned}$$

It is easy to see that

$$\int_0^\infty \iint_{\mathbb{R} \times \mathbb{R}} \left((S_t^* \psi_\varepsilon) * Q_t \right) (x) e^{ity} dE_B(x) K dE_A(y) dt = \int_0^\infty \left((S_t^* \psi_\varepsilon) * Q_t \right) (B) K \exp(itA) dt$$

and similar equalities hold for the other three integrals.

Thus

$$\begin{aligned} \psi_\varepsilon(B) - \psi_\varepsilon(A) - \frac{d}{ds} \left(\psi_\varepsilon(A_s) \right) \Big|_{s=0} &= \int_0^\infty \left(\left((S_t^* \psi_\varepsilon) * Q_t \right) (B) - \left((S_t^* \psi_\varepsilon) * Q_t \right) (A) \right) K \exp(itA) dt \\ &\quad + \int_0^\infty \left(\exp(itB) - \exp(itA) \right) K \left(\left((S_t^* \psi_\varepsilon) * Q_t \right) (A) \right) dt. \end{aligned}$$

We have

$$\lim_{\varepsilon \rightarrow 0} \left((S_t^* \psi_\varepsilon) * Q_t \right) (A) = \left((S_t^* \psi) * Q_t \right) (A)$$

in the strong operator topology (see the proof of Theorem 4 of [Pe1]). By Lemma 4.4,

$$\lim_{\varepsilon \rightarrow 0} \left(\left((S_t^* \psi_\varepsilon) * Q_t \right) (B) - \left((S_t^* \psi_\varepsilon) * Q_t \right) (A) \right) = \left((S_t^* \psi) * Q_t \right) (B) - \left((S_t^* \psi) * Q_t \right) (A)$$

in \mathbf{S}_2 .

It follows that

$$\begin{aligned} & \lim_{\varepsilon \rightarrow 0} \text{trace} \left(\left((S_t^* \psi_\varepsilon) * Q_t \right) (B) - \left((S_t^* \psi_\varepsilon) * Q_t \right) (A) \right) K \exp(itA) \\ &= \text{trace} \left(\left((S_t^* \psi) * Q_t \right) (B) - \left((S_t^* \psi) * Q_t \right) (A) \right) K \exp(itA) \end{aligned}$$

and

$$\begin{aligned} & \lim_{\varepsilon \rightarrow 0} \text{trace} \left(\left(\exp(itB) - \exp(itA) \right) K \left((S_t^* \psi_\varepsilon) * Q_t \right) (A) \right) \\ &= \text{trace} \left(\left(\exp(itB) - \exp(itA) \right) K \left((S_t^* \psi) * Q_t \right) (A) \right). \end{aligned}$$

Thus

$$\begin{aligned} & \lim_{\varepsilon \rightarrow 0} \text{trace} \left(\psi_\varepsilon(B) - \psi_\varepsilon(A) - \frac{d}{ds} \left(\psi_\varepsilon(A_s) \right) \Big|_{s=0} \right) \\ &= \int_0^\infty \text{trace} \left(\left((S_t^* \psi) * Q_t \right) (B) - \left((S_t^* \psi) * Q_t \right) (A) \right) K \exp(itA) dt \\ &+ \int_0^\infty \text{trace} \left(\left(\exp(itB) - \exp(itA) \right) K \left((S_t^* \psi) * Q_t \right) (A) \right) dt \\ &= \text{trace} \left(\psi(B) - \psi(A) - \frac{d}{ds} \left(\psi(A_s) \right) \Big|_{s=0} \right), \end{aligned}$$

which proves (4.1). ■

Proof of Lemma 4.4. We have

$$f_n(B) - f_n(A) = \iint_{\mathbb{R} \times \mathbb{R} \setminus \Delta} \check{f}_n(x, y) dE_B(x) K dE_A(y) = \iint_{\mathbb{R} \times \mathbb{R} \setminus \Delta} \check{f}_n(x, y) d\mathcal{E} K(x, y),$$

where \mathcal{E} is the spectral measure on the space \mathcal{S}_2 defined by $\mathcal{E}(\delta \times \sigma)T = E_B(\delta)TE_A(\sigma)$, $\delta, \sigma \subset \mathbb{R}$, $T \in \mathcal{S}_2$, and $\Delta \subset \mathbb{R} \times \mathbb{R}$ is the diagonal: $\Delta = \{(x, x) : x \in \mathbb{R}\}$. Then

$$\left\| (f_n(B) - f_n(A)) - (f(B) - f(A)) \right\|_{\mathcal{S}_2}^2 = \iint_{\mathbb{R} \times \mathbb{R} \setminus \Delta} |\check{f}_n(x, y) - \check{f}(x, y)|^2 d(\mathcal{E}K, K)(x, y) \rightarrow 0$$

as $n \rightarrow \infty$. ■

Now we are going to extend formula (4.1) to the whole class $B_{\infty 1}^2$. Consider first the case when φ is a polynomial of degree at most 2. Clearly, for linear functions φ the operator on the left-hand side of (4.1) is the zero operator and the right-hand side of (4.1) is equal to 0. Suppose now that $\varphi(t) = t^2$. If we perform formal manipulations, we

obtain

$$\begin{aligned} & (A + K)(A + K) - A^2 - \frac{d}{ds}(A + sK)(A + sK) \Big|_{s=0} \\ &= KA + AK + K^2 - \frac{d}{ds}(A^2 + sKA + sAK + s^2K^2) \Big|_{s=0} = K^2. \end{aligned}$$

We can put now by definition

$$(A + K)^2 - A^2 - \frac{d}{ds}(A + sK)^2 \Big|_{s=0} = K^2.$$

The following result establishes formula (4.1) for the function φ , $\varphi(t) = t^2$.

Theorem 4.5.

$$\text{trace } K^2 = 2 \int_{\mathbb{R}} \eta(x) dx. \quad (4.9)$$

Proof. To establish (4.9), we first assume that A is a bounded operator. Consider a sequence $\{g_n\}_{n \geq 1}$ such that

$$g_n(x) = x^2 \quad \text{for } x \in [-n, n], \quad \mathcal{F}g_n'' \in L^1, \quad \text{and} \quad \sup_{n \geq 1} \|\mathcal{F}g_n''\|_{L^1} < \infty.$$

Then for $n \geq \|A\| + \|K\|$ we have

$$\begin{aligned} \text{trace } K^2 &= \text{trace} \left(g_n(B) - g_n(A) - \frac{d}{ds}(g_n(A_s)) \Big|_{s=0} \right) \\ &= \int_{\mathbb{R}} g_n''(x) \eta(x) dx \rightarrow 2 \int_{\mathbb{R}} \eta(x) dx, \quad \text{as } n \rightarrow \infty. \end{aligned}$$

If A is an unbounded operator, consider the bounded self-adjoint operator A_n defined by

$$A_n = AE_A([-n, n]).$$

Let η_n be the generalized spectral shift function that correspond to the pair $(A_n, A_n + K)$. Then

$$\text{trace } K^2 = 2 \int_{\mathbb{R}} \eta_n(x) dx$$

and (4.9) follows from the fact that

$$\lim_{n \rightarrow \infty} \int_{\mathbb{R}} \eta_n(x) dx = \int_{\mathbb{R}} \eta(x) dx,$$

which can be found in [Ko1]. ■

Finally, we obtain the following result.

Theorem 4.6. *The map*

$$\varphi \mapsto \varphi(B) - \varphi(A) - \frac{d}{ds}(\varphi(A_s)) \Big|_{s=0}$$

extends from $B_{\infty 1}^2(\mathbb{R}) \cap \text{Lip}$ to a bounded linear operator from $B_{\infty 1}^2(\mathbb{R})$ to \mathcal{S}_1 and trace formula (4.1) holds for functions φ in $B_{\infty 1}^2(\mathbb{R})$.

Proof. Since the linear combinations of quadratic polynomials and functions whose Fourier transforms have compact support in $\mathbb{R} \setminus \{0\}$ are dense in $B_{\infty 1}^2(\mathbb{R})$, the result follows immediately from Theorems 4.3 and 4.5. ■

5. Open problems

The following interesting problems remain open.

Problem 1. Suppose that φ is a function of class C^2 on \mathbb{T} , U is a unitary operator, A is a self-adjoint operator of class \mathcal{S}_2 . Is it true that

$$\varphi(U_1) - \varphi(U) - \frac{d}{ds} \left(\varphi(U_s) \right) \Big|_{s=0} \in \mathcal{S}_1,$$

where $U_s = e^{isA}U$?

Problem 2. Suppose that $\varphi \in C^2(\mathbb{R})$ and $\varphi'' \in L^\infty$. Let A be a self-adjoint operator and let K be a self-adjoint operator of class \mathcal{S}_2 . Is it true that

$$\varphi(A_1) - \varphi(A) - \frac{d}{ds} \left(\varphi(A_s) \right) \Big|_{s=0} \in \mathcal{S}_1,$$

where $A_s = A + sK$?

Note that the right-hand sides of trace formulae (1.4) and (1.3) are well-defined for such functions. I conjecture that the answer to both questions should be negative.

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