IJMMS 25:4 (2001) 239–252
PII. S0161171201004318
http://ijmms.hindawi.com

KREĬN'S TRACE FORMULA AND THE SPECTRAL SHIFT FUNCTION

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(Received 15 October 1999 and in revised form 3 January 2000)

ABSTRACT. Let A,B be two selfadjoint operators whose difference $B-A$ is trace class. Kreĭn proved the existence of a certain function $\xi \in L_1(\mathbb{R})$ such that $\operatorname{tr}[f(B)-f(A)] = \int_{\mathbb{R}} f'(x)\xi(x)\,dx$ for a large set of functions f. We give here a new proof of this result and discuss the class of admissible functions. Our proof is based on the integral representation of harmonic functions on the upper half plane and also uses the Baker-Campbell-Hausdorff formula.

2000 Mathematics Subject Classification. Primary 47A55; Secondary 81Q05, 81U20.

1. Introduction. Kreĭn [19, 20, 21] developed the trace formula

$$\operatorname{tr}[f(B)-f(A)] = \int_{\mathbb{R}} f'(x)\xi(x)\,dx \tag{1.1}$$

which originated from Lifšic [22]. The function ξ is known as Kreĭn's spectral shift function (SSF) and has important applications in spectral theory. For instance, ξ is related to the scattering matrix $S(\lambda)$ for A and B by the remarkable formula [3],

$$\det S(\lambda) = e^{-2\pi i \xi(\lambda)}. \tag{1.2}$$

More recently, Kreĭn's spectral shift function was used for the computation of Witten's index in supersymmetric scattering theory [7, 14] and in inverse spectral theory for Schrödinger operators [15]. The trace formula can also be viewed as a mean value theorem for operators [10]. A comprehensive survey and references can be found in [6]. For more recent results see [4, 12, 13, 18, 29], and for extensions to non-selfadjoint operators see [1, 16, 26] and the references therein. Long time Kreĭn's original proof [19]—also in [2, 21, 28, 32]—was the only one available. This proof is based on the relation

$$\log\det{}_{B/A}(z) = \int_{\mathbb{R}} \frac{\xi(x)}{x-z}\,dx, \tag{1.3}$$

where $\det_{B/A}$ is the perturbation determinant for the pair A,B. It uses properties of such determinants and the integral representation of holomorphic functions on the upper half plane with a bounded imaginary part. In 1985, Voiculescu [31] approached the trace formula from a different direction. He constructed explicitly the spectral shift function in the finite dimensional case and then used the quasidiagonality of selfadjoint operators relative to the Hilbert-Schmidt class to extend by approximation the trace formula to bounded operators on a separable Hilbert space. Recently, Sinha and Mohapatra [28] applied a sophisticated approximation procedure to extend the formula from bounded to unbounded operators and thus provided an alternative proof of Kreĭn's theorem. Another approach, using contour integration was suggested in [27]. We highly recommend the recent article [4] which contains very interesting comments on several formula representations of the SSF.

Outline of the paper. We give here a new proof of the trace formula which does not use determinants or approximation. The spectral shift function is defined as the boundary value of one appropriate harmonic function on the upper half plane, see (2.6). This way we provide a new formula representation for the SSF. A special feature of our proof is the connection to the Baker-Campbell-Hausdorff formula in Lemma 1.1.

In Section 2, we state Kreĭn's theorem. Section 3 contains its proof. In Section 4, we give some examples of admissible functions and in Section 5, we deal with a substitution in the trace formula. The Baker-Campbell-Hausdorff formula is discussed in Section 6. The paper is accessible to graduate students with a background in functional analysis.

Prerequisite. We work with linear operators on a complex Hilbert space. Throughout S_1 stands for the trace class. The notation $\|\cdot\|_1$ is used for the norm on S_1 as well as for the norm on $L_1(\mathbb{R})$, and $\|\cdot\|$ is the uniform operator norm.

Lemma 1.1. *Let X,Y be two bounded operators with $X+Y\in S_1$. If $\|X\|,\|Y\|$ are sufficiently small, then the operator Z defined by $e^Xe^Y=e^Z$ belongs to the trace class, and*

$$\operatorname{tr} Z=\operatorname{tr}(X+Y). \tag{1.4}$$

The proof is given in Section 6.

We need some simple facts about Poisson integrals and harmonic functions which can be found, for instance, in [17].

Lemma 1.2. *For every $g\in L_1(\mathbb{R})$,*

$$g(x)=\lim_{y\to 0+}\frac{1}{\pi}\int_{\mathbb{R}}g(t)\frac{y}{y^2+(x-t)^2}\,dt \tag{1.5}$$

almost everywhere. The convergence is everywhere and uniform when g is uniformly continuous.

Lemma 1.3 (Fatou). *If $h(x,y)$, $x\in\mathbb{R}$, $y>0$ is a bounded harmonic function on the upper half plane, then its nontangential boundary values $h(x)=\lim_{y\to 0+}h(x,y)$ exist almost everywhere and*

$$h(x,y)=\frac{1}{\pi}\int_{\mathbb{R}}h(t)\frac{y}{y^2+(x-t)^2}\,dt. \tag{1.6}$$

2. Kreĭn's trace formula

Definition 2.1. Let K be the set of all functions with the representation

$$f(x) = \int_{\mathbb{R}} \frac{e^{isx} - 1}{s}\, d\mu(s), \tag{2.1}$$

where μ is a finite measure on $\mathbb{R}$.

If A is a selfadjoint operator with spectral resolution $E_A(\lambda)$ and $f \in K$, we define as usual

$$f(A) = \int_{\mathbb{R}} f(\lambda)\, dE_A(\lambda) = \int_{\mathbb{R}} \frac{e^{isA} - 1}{s}\, d\mu(s). \tag{2.2}$$

Lemma 2.2. *Suppose that A, B are selfadjoint operators and $B - A \in S_1$. Then for all $f \in K$:*

$$f(B) - f(A) \in S_1 \qquad \text{and} \qquad \|f(B) - f(A)\|_1 \le \|B - A\|_1 \|\mu\|. \tag{2.3}$$

Theorem 2.3. *Let A and B be two selfadjoint operators with $B - A \in S_1$. There exists a function $\xi \in L^1(\mathbb{R})$ such that*

(a) *for every $f \in K$,*

$$\operatorname{tr}[f(B) - f(A)] = \int_{\mathbb{R}} f'(x)\xi(x)\, dx. \tag{2.4}$$

In particular,

$$\operatorname{tr}(B - A) = \int_{\mathbb{R}} \xi(x)\, dx. \tag{2.5}$$

(b) $\|\xi\|_1 \le \|B - A\|_1$.

(c) *If $A \le B$, then $0 \le \xi$ almost everywhere.*

(d) $\xi(x) = 0$ *outside of any interval containing $\sigma(A) \bigcup \sigma(B)$.*

The function ξ is called Kreĭn's spectral shift function (SSF). It can be computed by the formula

$$\xi(x) = \lim_{y \to 0+} h(x, y), \quad \text{a.e. } x \in \mathbb{R}, \tag{2.6}$$

where

$$h(x, y) = \frac{1}{\pi} \operatorname{tr}\left[\arctan\frac{B - x}{y} - \arctan\frac{A - x}{y}\right] = \frac{1}{2\pi i} \int_{\mathbb{R}} e^{-ixs - y|s|} \operatorname{tr}\left[\frac{e^{isB} - e^{isA}}{s}\right] ds. \tag{2.7}$$

We write sometimes $\xi(x) = \xi(x; A, B)$ to indicate the dependence on A and B.

3. Proof of Theorem 2.3. First we prove Lemma 2.2. The relation

$$e^{isB} - e^{isA} = \int_0^s e^{i(s-t)B}(B - A)e^{itA}\, dt \tag{3.1}$$

implies

$$\left\|e^{isB} - e^{isA}\right\|_1 \le |s|\, \|B - A\|_1. \tag{3.2}$$

When $f \in K$, we have

$$f(B) - f(A) = \int_{\mathbb{R}} \frac{e^{isB} - e^{isA}}{s}\, d\mu(s). \tag{3.3}$$

Therefore $f(B)-f(A)\in S_1$ and

$$\|f(B)-f(A)\|_1 \le \int_{\mathbb{R}} \frac{\|e^{isB}-e^{isA}\|_1}{|s|}\,d|\mu|(s) \le \|B-A\|_1\|\mu\|. \tag{3.4}$$

We introduce one important tool, the function $g(t)=\arctan t$. It belongs to the class K because the two representations

$$\arctan t = \int_0^1 \frac{t}{1+t^2u^2}\,du, \quad \frac{t}{1+t^2u^2} = \frac{t}{2}\int_{\mathbb{R}} e^{itus}e^{-|s|}\,ds \tag{3.5}$$

together give

$$\arctan t = \frac{1}{2i}\int_{\mathbb{R}} \frac{e^{ist}-1}{s}e^{-|s|}\,ds. \tag{3.6}$$

For all $x\in\mathbb{R}$, $y>0$, we define

$$h(x,y) = \frac{1}{\pi}\operatorname{tr}\left[\arctan\frac{B-x}{y} - \arctan\frac{A-x}{y}\right]. \tag{3.7}$$

In view of (3.4) and (3.6),

$$\pi\,|h(x,y)| \le \left\|\arctan\frac{B-x}{y} - \arctan\frac{A-x}{y}\right\|_1 \le \frac{1}{y}\|B-A\|_1. \tag{3.8}$$

Using the representation (3.6) we can write also

$$h(x,y) = \frac{1}{2\pi i}\int_{\mathbb{R}} e^{-ixs-y|s|}\operatorname{tr}\left[\frac{e^{isB}-e^{isA}}{s}\right]ds \tag{3.9}$$

which shows that $h(x,y)$ is harmonic in the upper half plane $x\in\mathbb{R}$, $y>0$. To find out more about this function we study one special unitary operator.

Set $z=x+iy$ and consider the unitary Cayley transforms:

$$\begin{aligned} T_A &= (A-\bar{z})(A-z)^{-1} = I+2iy(A-z)^{-1}, \\ T_B &= (B-\bar{z})(B-z)^{-1} = I+2iy(B-z)^{-1}. \end{aligned} \tag{3.10}$$

Then define the unitary operator $U(x,y)=T_AT_B^*$ and compute

$$U-I = T_AT_B^* - T_BT_B^* = (T_A-T_B)T_B^* = i2y\left[(A-z)^{-1}-(B-z)^{-1}\right]T_B^* \tag{3.11}$$

which gives

$$U(x,y) = I+i2y(A-z)^{-1}(B-A)(B-\bar{z})^{-1}. \tag{3.12}$$

Suppose now that $B-A$ is a nonnegative one-dimensional operator:

$$B-A = \alpha\langle\cdot,w\rangle w, \quad \text{where } \alpha>0,\ \|w\|=1. \tag{3.13}$$

Then

$$U = I+i2y\alpha\langle\cdot,(B-z)^{-1}w\rangle(A-z)^{-1}w. \tag{3.14}$$

Taking $v=(A-z)^{-1}w$, we find

$$Uv = \left(1+i2y\alpha\langle(A-z)^{-1}w,(B-z)^{-1}w\rangle\right)v \tag{3.15}$$

which shows that U has an eigenvalue $1+\alpha(x,y)$ with

$$\alpha(x,y) = 2iy\alpha\langle (A-z)^{-1}w,(B-z)^{-1}w\rangle. \tag{3.16}$$

The unitary operator U has exactly two eigenvalues, 1 and $1+\alpha(x,y)$, as $B-A$ has exactly two eigenvalues, 0 and α. Because of this, $\alpha(x,y) \neq 0$ for all $x \in \mathbb{R}$, $y > 0$. If $\alpha(x,y) = 0$ for some x,y, then $U(x,y)$ has only one eigenvalue 1 and $U(x,y) = I$ which is impossible, since $A \neq B$. Therefore we can write

$$1+\alpha(x,y) = e^{i2\pi\theta(x,y)}, \tag{3.17}$$

where $\theta(x,y)$ is a continuous function on the upper half plane with $0 < \theta < 1$. The unitary operator U itself has the representation $U = e^{i2\pi H}$, with H a selfadjoint trace class operator, having two eigenvalues, 0 and θ. Using the logarithm with argument in $(0,2\pi)$, we can write

$$i2\pi H = \log U, \qquad i2\pi\theta = \operatorname{tr}\log U = \log\left(1+\alpha(x,y)\right). \tag{3.18}$$

Set

$$X = 2\arctan\frac{A-x}{y}, \qquad Y = 2\arctan\frac{B-x}{y}. \tag{3.19}$$

Spectral theory easily gives

$$T_A = e^{-iX}, \qquad T_B = e^{-iY}. \tag{3.20}$$

For large $y > 0$ the operators X,Y have small norms and by Lemma 1.1,

$$i2\pi\theta = \operatorname{tr}\log\left(e^{-iX}e^{iY}\right) = i\operatorname{tr}(Y-X) = i2\pi h, \tag{3.21}$$

that is, $\theta(x,y) = h(x,y)$. Since $\theta(x,y)$ is harmonic for large y, it is harmonic for all $y > 0$ because it has the same structure for all $y > 0$,

$$\theta(x,y) = \frac{1}{2\pi i}\log\left(1+2iy\alpha\langle (A-z)^{-1}w,(B-z)^{-1}w\rangle\right). \tag{3.22}$$

We conclude that $\theta(x,y) = h(x,y)$ on the whole upper half plane because both functions are defined and harmonic there. Therefore $0 < h < 1$. By Fatou's theorem it has boundary values $\xi(x) = \lim_{y\to 0+} h(x,y)$ a.e. with $0 \le \xi \le 1$ and

$$h(x,y) = \frac{1}{\pi}\int_{\mathbb{R}} \frac{y}{y^2+(x-t)^2}\xi(t)\,dt. \tag{3.23}$$

From (3.8),

$$\lim_{y\to\infty} \pi y h(x,y) = \int_{\mathbb{R}} \xi(t)\,dt = \|\xi\|_1 \le \|B-A\|_1. \tag{3.24}$$

When $\alpha < 0$ we can change the places of A,B and define $\xi(t;B,A) = -\xi(t;A,B) \ge 0$, so that in this case $\xi(t;A,B) \le 0$. For completeness, if $\alpha = 0$ we set $\xi(t;A,B) = 0$.

In order to define ξ for an arbitrary trace class perturbation

$$B-A=\sum_{k=1}^{\infty}\alpha_k\langle\cdot,w_k\rangle w_k,\qquad \|B-A\|_1=\sum_{k=1}^{\infty}|\alpha_k|<\infty, \tag{3.25}$$

we proceed by the staircase method. Let

$$B_n=A+\sum_{k=1}^{n}\alpha_k\langle\cdot,w_k\rangle w_k,\qquad \lim_{n\to\infty}\|B-B_n\|_1=0. \tag{3.26}$$

Suppose that we have defined $\xi(t;A,B_n)$ for some n with

$$\begin{gathered}\|\xi(t;A,B_n)\|_1\le\|B_n-A\|_1,\\ \operatorname{tr}\left[\arctan\frac{B_n-x}{y}-\arctan\frac{A-x}{y}\right]=\int_{\mathbb{R}}\frac{y}{y^2+(x-t)^2}\xi(t;A,B_n)\,dt.\end{gathered} \tag{3.27}$$

Then we set

$$\xi(t;A,B_{n+1})=\xi(t;A,B_n)+\xi(t;B_n,B_{n+1}), \tag{3.28}$$

$$\|\xi(t;A,B_{n+1})\|_1\le\|\xi(t;A,B_n)\|_1+\|\xi(t;B_n,B_{n+1})\|_1\le\sum_{k=1}^{n+1}|\alpha_k|=\|B_{k+1}-A\|_1 \tag{3.29}$$

and (3.27) holds for $n+1$ because we can add and subtract $\arctan[(B_{n+1}-x)/y]$ in the left-hand side. By induction, the functions $\xi(t;A,B_n)$ are defined for all n and it is trivial to see that they form a Cauchy sequence in $L^1(\mathbb{R})$. The limit

$$\xi(t)=\xi(t;A,B)=\lim\xi(t;A,B_n) \tag{3.30}$$

exists with $\|\xi(t)\|_1\le\|B-A\|_1$.

Proof of (c). When $B-A\ge0$, then all $\alpha_k\ge0$ and in view of (3.28) we find by induction $\forall n:\xi(t;A,B_n)\ge0$. Therefore $\xi\ge0$. □

Proof of (a). By (3.4), the following estimate is true

$$\left\|\arctan\frac{B-x}{y}-\arctan\frac{B_n-x}{y}\right\|_1\le\frac{1}{y}\|B-B_n\|_1. \tag{3.31}$$

□

Passing to limits in (3.27), we find

$$\operatorname{tr}\left[\arctan\frac{B-x}{y}-\arctan\frac{A-x}{y}\right]=\int_{\mathbb{R}}\frac{y}{y^2+(x-t)^2}\xi(t)\,dt. \tag{3.32}$$

This relation, true for all $x\in\mathbb{R}$, $y>0$ implies

$$\operatorname{tr}[f(B)-f(A)]=\int_{\mathbb{R}}f'(t)\xi(t)\,dt \tag{3.33}$$

for all functions $f\in K$. Indeed, given $f(t)=\int_{\mathbb{R}}(e^{ist}-1)/s\,d\mu(s)$ define

$$f(t;y)=\int_{\mathbb{R}}\frac{e^{ist}-1}{s}e^{-y|s|}\,d\mu(s),\quad y>0. \tag{3.34}$$

We have

$$\begin{aligned}\frac{d}{dt}f(t;y) = f'(t;y) &= i\int_{\mathbb{R}} e^{ist}e^{-y|s|}\,d\mu(s)\\ &= i\int_{\mathbb{R}}\left[\frac{1}{\pi}\int_{\mathbb{R}}\frac{y}{y^2+(x-t)^2}e^{isx}\,dx\right]d\mu(s)\\ &= \frac{1}{\pi}\int_{\mathbb{R}}\frac{y}{y^2+(x-t)^2}\left[i\int_{\mathbb{R}}e^{isx}\,d\mu(s)\right]dx\\ &= \frac{1}{\pi}\int_{\mathbb{R}}\frac{y}{y^2+(x-t)^2}f'(x)\,dx.\end{aligned} \tag{3.35}$$

Integrating for t and adjusting the constant of integration so that $f(0,y)=0$, we find

$$f(t;y) = \frac{1}{\pi}\int_{\mathbb{R}}\left[\arctan\frac{t-x}{y}+\arctan\frac{x}{y}\right]f'(x)\,dx \tag{3.36}$$

therefore,

$$\begin{aligned}\operatorname{tr}[f(B;y)-f(A;y)] &= \frac{1}{\pi}\int_{\mathbb{R}}\operatorname{tr}\left[\arctan\frac{B-x}{y}-\arctan\frac{A-x}{y}\right]f'(x)\,dx\\ &= \int_{\mathbb{R}}\left[\frac{1}{\pi}\int_{\mathbb{R}}f'(x)\frac{y}{y^2+(x-t)^2}\,dx\right]\xi(t)\,dt.\end{aligned} \tag{3.37}$$

Taking limits for $y\to 0+$ we come to (3.33).

The limit

$$\lim_{y\to 0+}\operatorname{tr}[f(B;y)-f(A;y)] = \operatorname{tr}[f(B)-f(A)] \tag{3.38}$$

becomes obvious when we compare

$$\operatorname{tr}[f(B;y)-f(A;y)] = \int_{\mathbb{R}}\operatorname{tr}\left[\frac{e^{isB}-e^{isA}}{s}\right]e^{-y|s|}\,d\mu(s) \tag{3.39}$$

with

$$\operatorname{tr}[f(B)-f(A)] = \int_{\mathbb{R}}\operatorname{tr}\left[\frac{e^{isB}-e^{isA}}{s}\right]d\mu(s). \tag{3.40}$$

The function $f(t)=t$ belongs to K with $d\mu(s) = -i\delta(s)ds$. This gives

$$\operatorname{tr}(B-A) = \int_{\mathbb{R}}\xi(t)\,dt. \tag{3.41}$$

Proof of (d). Suppose $\sigma(A)\bigcup\sigma(B)\subseteq[a,b]$ and $x<a$. The relation

$$\arctan t = \frac{\pi}{2}-\arctan\frac{1}{t}\quad (t>0) \tag{3.42}$$

gives (by using the spectral theorem with integration over $(-\infty,x]$ and $[x,+\infty)$)

$$\arctan\frac{B-x}{y}-\arctan\frac{A-x}{y} = \arctan[y(A-x)^{-1}]-\arctan[y(B-x)^{-1}]. \tag{3.43}$$

Therefore,

$$\xi(x) = \lim_{y\to 0+}\frac{1}{\pi}\operatorname{tr}[\arctan(y(A-x)^{-1})-\arctan(y(B-x)^{-1})] = 0. \tag{3.44}$$

The case $x > b$ is treated similarly, using the relation

$$\arctan t = -\frac{\pi}{2} - \arctan\frac{1}{t} \quad (t < 0). \tag{3.45}$$

Moreover, if the spectra of the operators are separated, it easily follows that on intervals between them the SSF is a constant. The proof is completed. □

Remark 3.1. The above proof allows a natural extension of Kreĭn's formula. Let A and B be the generators of one-parameter C_0-groups of operators: e^{itA}, e^{itB}, $t \in \mathbb{R}$, of at most polynomial growth

$$\|e^{itA}\|, \|e^{itB}\| \le M(1+|t|)^{\alpha}, \quad \alpha \ge 0 \tag{3.46}$$

(when $M = 1$, $\alpha = 0$, the operators are selfadjoint). The harmonic function (3.7) is well defined and its boundary value (2.6) is a certain distribution for which (2.4) holds.

4. Admissible functions. Let A, B be two selfadjoint operators with $B - A \in S_1$. One differentiable function $f(x)$ defined on some interval containing $\sigma(A) \bigcup \sigma(B)$ is called *admissible*, if $f(B) - f(A) \in S_1$ and the trace formula (2.4) holds. We proved that the functions in the set K are admissible. Obviously, if f is admissible, then $f + c$ is also admissible for any constant c. Any linear combination of admissible functions is admissible. One could expect that every function with $f' \in L_\infty(\mathbb{R})$ is admissible. However, Farforovskaya produced an example of a function f with bounded continuous derivative and a pair of selfadjoint operators A, B such that $B - A \in S_1$ but $f(B) - f(A) \notin S_1$ (see [11] and the note at the end of it). The characterization of all admissible functions is an open problem. Birman and Solomyak [5], using the methods of double operator integrals, described a large class of admissible functions, including those with $f' \in L_p(\mathbb{R}) \bigcap \mathrm{Lip}\,\epsilon$, where $1 \le p < \infty$, $\epsilon > 0$. Their investigations were continued by Peller [24, 25], who showed that every function in the Besov class $B^1_{\infty,1}$ is admissible. Using only simple means, we want to give here some examples of admissible functions, besides those in K.

Proposition 4.1 [20]. *Suppose $v(t)$ is a finite measure on a set $M \subseteq \mathbb{R}$ such that*

$$\int_M |t|\,d|v|(t) < \infty. \tag{4.1}$$

Then all functions of the form $f(x) = \int_M e^{itx}\,dv(t)$ are admissible.

Proof. Writing the trace formula for the admissible function

$$f_t(x) = \frac{e^{itx} - 1}{t} \tag{4.2}$$

we get

$$\operatorname{tr}\left(e^{itB} - e^{itA}\right) = \int_{\mathbb{R}} ite^{itx}\xi(x)\,dx \tag{4.3}$$

which shows that the function $g_t(x) = e^{itx}$ is admissible. In view of (3.2), we can multiply both sides in (4.3) by dv and integrate over M. □

Corollary 4.2. *When* $\operatorname{Im}(z) \neq 0$ *the function* $f_z(x) = 1/(x+z)$ *and all its derivatives are admissible.*

Proof. Let $z = s + it$. For $t > 0$, we write

$$\frac{1}{x+s+it} = \frac{-i}{-ix-is+t} = -i\int_0^\infty e^{i\lambda x}e^{i\lambda s}e^{-\lambda t}\,d\lambda \tag{4.4}$$

and for $t < 0$,

$$\frac{1}{x+s+it} = \frac{i}{ix+is-t} = i\int_0^\infty e^{-i\lambda x}e^{-is\lambda}e^{\lambda t}\,d\lambda. \tag{4.5}$$

The result follows immediately from here. We deduce that the function

$$f_t(x) = \frac{x}{x^2+t^2} = \frac{1}{2}\left[\frac{1}{x+it} + \frac{1}{x-it}\right] \tag{4.6}$$

is also admissible.

Now we turn to the case of nonnegative operators A, B. In view of property (d) we need to consider only functions on $[0,\infty)$. □

Proposition 4.3. *Let* $0 \le A, B$ *and* $\nu(t)$ *be a finite measure on* $[0,\infty)$ *with*

$$\int_0^\infty |t|d|\nu|(t) < \infty. \tag{4.7}$$

Then all functions of the form

$$f(x) = \int_0^\infty e^{-tx}\,d\nu(t), \quad x \ge 0, \tag{4.8}$$

are admissible.

Proof. When $t, x > 0$ the function $f_t(x) = e^{-tx}$ is admissible, as seen from

$$e^{-tx} = 1 + \frac{t^2}{\pi}\int_{\mathbb{R}} \frac{e^{-isx}-1}{is}\frac{ds}{t^2+s^2} \tag{4.9}$$

(to check this, differentiate both sides for x). Then one proceeds as in Proposition 4.1, integrating

$$\operatorname{tr}(e^{-tB} - e^{-tA}) = -\int_0^\infty te^{-tx}\xi(x)\,dx. \tag{4.10}$$

□

Proposition 4.4. *Suppose* $0 < \epsilon I \le A, B$ *and* $f(x)$ *is a function on* $(0,\infty)$ *that admits a bounded holomorphic extension* $f(z)$ *on the right half plane* $\operatorname{Re}(z) > 0$*. Then* f *is admissible for* A, B*.*

Proof. One has the Poisson representation

$$f(x) = \frac{1}{\pi}\int_{\mathbb{R}} f(it)\frac{x}{x^2+t^2}\,dt, \tag{4.11}$$

where $f(it)$ is the boundary value of $f(z)$ defined a.e. The spectral theorem gives

$$f(A) = \frac{1}{\pi}\int_{\mathbb{R}} f(it)\frac{A}{A^2+t^2}\,dt. \tag{4.12}$$

In the same way we represent $f(B)$. Since the function $x/(x^2+t^2)$ is admissible, one can write

$$\operatorname{tr}\left[\frac{B}{B^2+t^2}-\frac{A}{A^2+t^2}\right]=\int_{\mathbb{R}}\frac{t^2-x^2}{(x^2+t^2)^2}\xi(x)\,dx. \tag{4.13}$$

Multiplying both sides by $f(it)$ and integrating over $\mathbb{R}$ one comes to (2.4). To see that the integral on the left side converges, one needs to check that $f(B)-f(A)\in S_1$. Indeed,

$$\begin{aligned}\left\|\frac{1}{B+it}-\frac{1}{A+it}\right\|_1&=\left\|\frac{1}{B+it}(B-A)\frac{1}{A+it}\right\|_1\\&\le\left\|\frac{1}{B+it}\right\|\left\|\frac{1}{A+it}\right\|\|B-A\|_1\le\frac{1}{(\epsilon+|t|)^2}\|B-A\|_1.\end{aligned} \tag{4.14}$$

Using the decomposition (4.6), one estimates

$$\left\|\frac{B}{B^2+t^2}-\frac{A}{A^2+t^2}\right\|_1\le\frac{1}{(\epsilon+|t|)^2}\|B-A\|_1 \tag{4.15}$$

and therefore,

$$\|f(B)-f(A)\|_1\le\frac{2}{\pi\epsilon}\sup_{\operatorname{Re}(z)>0}|f(z)|\|B-A\|_1. \tag{4.16}$$

$\square$

Example 4.5. Taking $f(x)=x^{is}$, $s\in\mathbb{R}$, one finds

$$\operatorname{tr}(B^{is}-A^{is})=is\int_{\epsilon}^{\infty}x^{is-1}\xi(x)\,dx. \tag{4.17}$$

Remark 4.6. In Proposition 4.4, one may assume only that $f(x)$ admits a bounded holomorphic extension on some sector $|\operatorname{Arg}(z)|<\pi/2$. The estimate (4.16) can be improved by using an appropriate integral representation of such function [9].

5. Φ-compatible operators. It may happen that the difference $B-A$ is not trace class, but for some common regular point z,

$$(B-z)^{-1}-(A-z)^{-1}\in S_1. \tag{5.1}$$

Such operators are called resolvent compatible. If (5.1) is true for some $z\in\rho(A)\bigcap\rho(B)$, then it is true for all $\lambda\in\rho(A)\bigcap\rho(B)$, as follows from the identity

$$(B-\lambda)^{-1}-(A-\lambda)^{-1}=(B-z)(B-\lambda)^{-1}\left[(B-z)^{-1}-(A-z)^{-1}\right](A-z)(A-\lambda)^{-1}. \tag{5.2}$$

An important case is when the operators are bounded from below. We may assume that $0\le A,B$. Then (5.1) is equivalent to

$$(B+I)^{-1}-(A+I)^{-1}\in S_1 \tag{5.3}$$

and we can apply the trace formula to the operators $(B+I)^{-1}$ and $(A+I)^{-1}$. After that the substitution $t\to t^{-1}-1$ brings to a trace formula for A,B.

More generally, we have the following.

Definition 5.1. Let Φ be a real-valued continuous function on some finite or infinite interval $[a,b]$ with Φ' existing and nonzero on (a,b). Two selfadjoint operators A,B with spectra in $[a,b]$ are called Φ-compatible, if

$$\Phi(B)-\Phi(A)\in S_1. \tag{5.4}$$

Kreĭn's trace formula extends to such operators by a simple substitution.

Corollary 5.2. *Suppose Φ is as above and A,B are Φ-compatible. There exists a spectral shift function ξ defined a.e. on $[a,b]$ for which*

$$\operatorname{tr}[f(B)-f(A)]=\int_a^b f'(t)\xi(t)\,dt \tag{5.5}$$

for any differentiable function f on $[a,b]$ such that $f(\Phi^{-1}(x))$ is admissible for the interval $[\Phi(a),\Phi(b)]$. *Property (d) stays the same, while (b) turns into*

$$\int_a^b |\xi(t)\Phi'(t)|\,dt\le \|\Phi(B)-\Phi(A)\|_1. \tag{5.6}$$

Proof. Write the trace formula (2.6) for the pair $\Phi(A),\Phi(B)$ and define

$$\xi(t)=\xi(\Phi(t);\Phi(A);\Phi(B)). \tag{5.7}$$

Then the substitution $x=\Phi(t)$ brings to (5.5). □

6. Proof of Lemma 1.1 (the Baker-Campbell-Hausdorff formula). It is known that if $X,Y\in B(H)$, then an infinite series $Z=Z(X,Y)$ exists such that

$$e^Z=e^Xe^Y. \tag{6.1}$$

For instance (see [8, Chapters 1 and 2], [23, 30]),

$$Z=X+Y+\sum_{n\ge 2}\frac{1}{n}\sum_{|w|=n} g_w[w], \tag{6.2}$$

where g_w are certain coefficients and $w=w_1w_2\cdots w_n$ is a "word" with length $|w|=n$, $n=2,3,\dots$, such that each w_K equals X or Y. Also, $[w]$ is the iterated commutator

$$[w]=[[\cdots[[w_1,w_2],w_3]\cdots],w_n]. \tag{6.3}$$

This series was studied by Thompson [30], who proved its convergence when X,Y have small norms. Details and precise statements can be found in his paper (see also [23]). A modification of Thompson's proof yields the following.

Proof of Lemma 1.1. If $X+Y\in S_1$, then $[X,Y]\in S_1$ too and $\operatorname{tr}[X,Y]=0$, as $[X,Y]=[X+Y,Y]$. The trace of all higher commutators is also zero. Now recall that $\|AB\|_1\le\|A\|\|B\|_1$ for any two operators $A\in B(H)$, $B\in S_1$. We set $\delta=\max\{\|X\|,\|Y\|\}$ and estimate

$$\begin{gathered}\|[X,Y]\|_1=\|[X+Y,Y]\|_1\le 2\|Y\|\|X+Y\|_1\le 2\delta\|X+Y\|_1,\\ \|[[X,Y],X]\|_1\le 2\|X\|\|[X,Y]\|_1\le 2^2\delta^2\|X+Y\|_1\end{gathered} \tag{6.4}$$

and so forth. By induction, for every $n \geq 2$,

$$\|[w]\|_1 \leq 2^{n-1}\delta^{n-1}\|X+Y\|_1 \tag{6.5}$$

whenever $|w| = n$. Combining this with Thompson's estimates [30, pages 5 and 6], we find

$$\left\| \sum_{|w|=n} g_w[w] \right\|_1 \leq 2^n \delta^{n-1}\|X+Y\|_1. \tag{6.6}$$

The series in (6.2) is majorized in the norm of S_1 by

$$\|X+Y\|_1 \sum_{n\geq 2} \frac{2^n\delta^{n-1}}{n} \tag{6.7}$$

which is convergent, since $\delta < 1/2$. Therefore, the expansion (6.2) converges in S_1 and the proof is completed. □

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