

TRACE FORMULA FOR NONNUCLEAR PERTURBATIONS OF SELFADJOINT OPERATORS

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Abstract. The trace formulas for the operator $\varphi(H_1) - \varphi(H_0)$ are deduced when $H_1 - H_0$ is a nonnuclear operator and φ is an enough wide class of functions.

1. Introduction. Suppose $B(\mathcal{H})$ is the algebra of all bounded operators over the Hilbert space $\mathcal{H}$. Denote by C_p and $|\cdot|_p$ the Neumann-Schatten class of operators and their norm [2]. For an operator $W \in C_2$ by $\det_2(I + W)$ we denote its regularized determinant.

Let H_1 and H_0 be selfadjoint operators (possibly unbounded) on a Hilbert space $\mathcal{H}$. If $H_1 - H_0 = V$ is a nuclear operator and φ is an element in a sufficiently large class of functions, then Krein [3,4] proved that $\varphi(H_1) - \varphi(H_0)$ is a nuclear operator and that

$$\text{trace } (\varphi(H_1) - \varphi(H_0)) = \int_R \xi(\lambda) \varphi'(\lambda) d\lambda, \quad (1.1)$$

where ξ is the real function in $L^1(R)$ uniquely determined by H_0 and H_1 . Usually, the relation (1.1) is called the trace formula.

Krein also proved the following relation between the function and the perturbation determinant:

$$\det(I + V(H_0 - z)^{-1}) = \exp \left(\int_R \frac{\xi(\lambda)}{\lambda - z} d\lambda \right), \quad \text{Im} z \neq 0.$$

Koplienko [5] extended the trace formula (1.1) to the case when $H_1 - H_0$ is not a nuclear operator. The trace formula was deduced when φ is a rational function with the poles in $C \setminus R$ and $|\varphi(\infty)| < \infty$.

In this paper we prove regularized trace formulas for a nonnuclear perturbation of selfadjoint operators in the case when φ is not an analytic function. Our method is different from the method given in [6]. The following theorem is a result of Koplienko:

THEOREM 1.1 *Let H_0, V be selfadjoint operators, $V \in C_2$ and let φ be a rational function with poles lying in $C \setminus R$ and $|\varphi(\infty)| < \infty$. Then*

- (1) $R_2 = \varphi(H_0 + V) - \varphi(H_0) - \frac{d}{dx}\varphi(H_0 + xV)|_{x=0} \in C_1$
- (2) *There exists a real function σ (depending only on H_0 and V) of bounded variation such that*

$$\text{trace } R_2 = \int_R \varphi''(\lambda) d\sigma(\lambda)$$

- (3) $V_{-\infty}^\infty \sigma \leq |V|_2^2/2!$ ($V_{-\infty}^\infty f$ is the variation of f on $(-\infty, \infty)$).

- (4) $\det_2(I + V(H_0 - z)^{-1}) = \exp\left(-\int_R \frac{d\sigma(\lambda)}{(\lambda - z)^2}\right).$

2. Results. Let $\mathcal{M}_p$ be the set of all the functions φ of the form $\varphi(x) = \int_R e^{itx} g(t) dt$ where g is a measurable function such that $\int_R |t|^\nu |g(t)| dt < \infty$ for $\nu = 0, 1, 2, \dots, p$ ($p \geq 2$). The functions from $\mathcal{M}_p$ are not necessarily analytic, and the set $\mathcal{M}_p$ contains the class of functions from Theorem 1.

Recall that if $A, B \in B(\mathcal{H})$, then [1] we have

$$e^{(A+B)t} = e^{A \cdot t} + \sum_{n=1}^{\infty} \int_0^t \int_0^{s_1} \dots \int_0^{s_{n-1}} e^{A(t-s_1)} B e^{A(s_1-s_2)} B \dots B e^{A(s_{n-1}-s_n)} B e^{A s_n} ds_1 ds_2 \dots ds_n \quad (2.0.1)$$

(The series converges in $B(\mathcal{H})$).

LEMMA 2.1 *If $H_0 = H_0^*$, $V = V^* \in B(\mathcal{H})$, $t, x \in R$, then*

$$e^{it(H_0+xV)} = e^{itH_0} + \sum_{n=1}^{\infty} i^n x^n B_n(t), \quad (2.1.1)$$

where

$$B_n(t) = \int_0^t \int_0^{s_1} \dots \int_0^{s_{n-1}} e^{iH_0(t-s_1)} V e^{iH_0(s_1-s_2)} V \dots V e^{iH_0(s_{n-1}-s_n)} V e^{iH_0 s_n} ds_1 ds_2 \dots ds_n \quad (2.1.2)$$

Proof. If $H_0 \in B(\mathcal{H})$, then (2.11) and (2.12) follow directly from (2.01). So, suppose that H_0 is an unbounded operator. Set $H^{(k)} = H_0 E(-k, k)$, where E is the spectral measure of H_0 . The operator $H^{(k)}$ is bounded and we have

$$\lim_{k \rightarrow \infty} \left(\lambda - H^{(k)} \right)^{-1} h = (\lambda - H_0)^{-1} h \quad (h \in \mathcal{H}, \text{Im} \lambda \neq 0)$$

i.e. the sequence $H^{(k)}$ converges to H_0 in the strong resolvent sense. By the Trotter Theorem [7] we have

$$\lim_{k \rightarrow \infty} e^{itH^{(k)}} h = e^{itH_0} h, \quad h \in \mathcal{H}, \quad t \in R. \quad (2.1.3)$$

Setting $H^{(k)}$ instead of H_0 in (2.1.1), (2.1.2) and letting k tend to infinity, we complete the proof of Lemma 1.

LEMMA 2.2 *If $H_0 = H_0^*$, $V = V^* \in B(\mathcal{H})$, $x, t \in R$, then for $k = 0, 1, 2, \dots$ the following inequality holds*

$$\left\| \frac{d^k}{dx^k} e^{it(H_0 + xV)} \right\| \leq |t|^k \|V\|^k. \quad (2.2.1)$$

Proof. Since

$$\frac{d^k}{dx^k} e^{it(H_0 + xV)} = \frac{d^k}{d\xi^k} e^{it(H_1 + \xi V)}|_{\xi=0} \quad (H_1 = H_0 + xV),$$

by Lemma 2.1, it follows

$$\frac{d^k}{d\xi^k} e^{it(H_1 + \xi V)}|_{\xi=0} = i^k k! \int_0^t \int_0^{s_1} \dots \int_0^{s_{n-1}} e^{iH_1(t-s_1)} V \dots V e^{iH_1 s_n} ds_1 ds_2 \dots ds_n$$

From the previous equality we have

$$\left\| \frac{d^k}{dx^k} e^{it(H_0 + xV)} \right\| \leq k! \int_0^t \int_0^{s_1} \dots \int_0^{s_{n-1}} \|V\|^k ds_1 ds_2 \dots ds_n = |t|^k \|V\|^k, \quad (t > 0)$$

and the proof is complete.

LEMMA 2.3 *If $H_0 = H_0^*$, $x, t \in R$, $V = V^* \in B(\mathcal{H})$ and $\varphi \in \mathcal{M}_p$ (i.e. $\varphi(x) = \int_R e^{itx} g(t) dt$, g is a measurable function), then*

$$\frac{d^k}{dx^k} \varphi(H_0 + xV) = \int_R \frac{d^k}{dx^k} e^{it(H_0 + xV)} g(t) dt. \quad (2.3.1)$$

Proof. For $k = 0$, (2.3.1) follows from the spectral theorem. If $k = 1$ we have

$$\frac{d}{dx} \varphi(H_0 + xV) = \lim_{\xi \rightarrow \infty} \int_R \frac{e^{it(H_0 + (x+\xi)V)} - e^{it(H_0 + xV)}}{\xi} g(t) dt. \quad (2.3.2)$$

Since

$$e^{it(H_0 + x_2 V)} - e^{it(H_0 + x_1 V)} = \int_{x_1}^{x_2} \frac{\partial}{\partial x} e^{it(H_0 + xV)} dx$$

by Lemma 2.2 we obtain

$$\left\| e^{it(H_0+x_2V)} - e^{it(H_0+x_1V)} \right\| \leq |t| \|V\| |x_2 - x_1|. \quad (2.3.3)$$

From (2.3.2), (2.3.3) and $\int_R |t| |g(t)| dt < \infty$, by the Theorem of Dominated Convergence, we conclude that

$$\frac{d}{dx} \varphi(H_0 + xV) = \int_R \frac{d}{dx} e^{it(H_0+xV)} g(t) dt.$$

Repeating this procedure several times we prove Lemma 2.3.

From now on we assume $V = V^* \in C_p$ ($p \geq 2$, $p \in N$).

LEMMA 2.4 *If $x, t \in R$, $H_0 = H_0^*$, then $\frac{d^p}{dx^p} e^{it(H_0+xV)}$ is a nuclear operator and*

$$\left| \frac{d^p}{dx^p} e^{it(H_0+xV)} \right|_1 \leq |t|^p |V|_p^p.$$

Proof. Since

$$\begin{aligned} \frac{d^p}{dx^p} e^{it(H_0+xV)} &= i^p p! \int_0^t \int_0^{s_1} \dots \int_0^{s_{p-1}} \\ &\quad e^{iH_1(t-s_1)} V \dots V e^{iH_1(s_{p-1}-s_p)} V e^{iH_1 s_p} ds_1 ds_2 \dots ds_p \end{aligned}$$

($H_1 = H_0 + xV$) and $V \in C_p$ we get $\frac{d^p}{dx^p} e^{it(H_0+xV)} \in C_1$ and

$$\left| \frac{d^p}{dx^p} e^{it(H_0+xV)} \right| \leq p! |V|_p^p \int_0^t \int_0^{s_1} \dots \int_0^{s_{p-1}} ds_1 ds_2 \dots ds_p = t^p |V|_p^p \quad (t > 0).$$

Set

$$U_p(t) = e^{it(H_0+V)} - \sum_{k=0}^{p-1} \frac{1}{k!} \frac{d^k}{dx^k} e^{it(H_0+xV)} \Big|_{x=0}$$

Now, by Lemma 2.3

$$R_p \stackrel{\text{def}}{=} \varphi(H_0 + V) - \sum_{k=0}^{p-1} \frac{1}{k!} \frac{d^k}{dx^k} \varphi(H_0 + xV) \Big|_{x=0} = \int_R U_p(t) g(t) dt.$$

LEMMA 2.5 *If $H_0 = H_0^*$, $V = V^* \in C_p$, $t \in R$, then $U_p(t) \in C_1$, $R_p \in C_1$ and*

$$\text{trace } R_p = \int_R g(t) \text{ trace } U_p(t) dt \quad (2.5.1)$$

Proof. Let $m(x) = e^{it(H_0 + xV)}$, (where t is a fixed real number and $x \in R$). By the Taylor theorem we obtain

$$m(1) = \sum_{\nu=0}^{p-1} \frac{m^{(\nu)}(0)}{\nu!} + \frac{1}{(p-1)!} \int_0^1 m^{(p)}(x)(1-x)^{p-1} dx$$

i.e.

$$U_p(t) = \frac{1}{(p-1)!} \int_0^1 m^{(p)}(x)(1-x)^{p-1} dx$$

Since $m^{(p)}(x) \in C^1$ (by Lemma 2.4) and $m^{(p)}$ is a continuous function in C_1 norm, we have $U_p(t) \in C_1$ ($\forall t \in R$). By Lemma 2.4 we get

$$|U_p(t)|_1 \leq \frac{1}{(p-1)!} \int_0^1 |m^{(p)}(x)|_1 (1-x)^{p-1} dx \leq \frac{1}{(p-1)!} \int_0^1 |t|^p |V|_p^p (1-x)^{p-1} dx$$

i.e.

$$|U_p(t)|_1 \leq |V|_p^p |t|^p / p!. \quad (2.5.2)$$

Hence R_p is a compact operator.

Let S be a unitary operator and suppose $\{e_i\}$ is an orthonormal set. Then

$$\begin{aligned} \left| \sum_{i=1}^r (SR_p e_i, e_i) \right| &= \left| \sum_{i=1}^r \left(\int_R g(t) S U_p(t) e_i, e_i \right) dt \right| = \left| \int_R g(t) \sum_{i=1}^r (S U_p(t) e_i, e_i) dt \right| \\ &\leq ([2]) \leq \int_R |g(t)| \sum_{i=1}^r s_i(U_p(t)) dt \leq \int_R |g(t)| |U_p(t)|_1 dt \\ &\leq \int_R |g(t)| |t|^p dt \cdot \frac{|V|_p^p}{p!}. \end{aligned} \quad (\text{by 2.5.2})$$

So,

$$\left| \sum_{i=1}^r (SR_p e_i, e_i) \right| \leq \frac{|V|_p^p}{p!} \int_R |t|^p |g(t)| dt.$$

When we take the supremum over all unitary operators S and over all orthonormal sets $\{e_i\}$, we obtain

$$\sum_{i=1}^r s_i(R_p) \leq \frac{|V|_p^p}{p!} \int_R |t|^p |g(t)| dt,$$

i.e.

$$R_p \in C_1, \quad |R_p|_1 \leq \frac{|V|_p^p}{p!} \int_R |t|^p |g(t)| dt \quad \text{and} \quad \text{trace } R_p = \int_R g(t) \text{ trace } U_p(t) dt.$$

This completes the proof

LEMMA 2.6 *If $H_0 = H_0^* \in B(\mathcal{H})$, $V = V^* \in C_p$ and $\Gamma = \{\lambda: |\lambda| = 1 + \|H_0\| + \|V\|\}$, then*

$$U_p(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{i\lambda t} G_p(\lambda) d\lambda$$

where $G_p(\lambda) = (\lambda - H_0)^{-1} (V(\lambda - H_0)^{-1})^p (I - V(\lambda - H_0)^{-1})^{-1}$

Proof. From $H_0 = H_0^*$ we have $\|V(\lambda - H_0)^{-1}\| \leq \|V\|(1 + \|V\|)^{-1} < 1$ for every $\lambda \in \Gamma$. Hence $(\lambda - H_0 - xV)^{-1} = \sum_{k=0}^{\infty} x^k (\lambda - H_0)^{-1} (V(\lambda - H_0)^{-1})^k$; it follows that

$$\frac{d^k}{dx^k} (\lambda - H_0 - xV)^{-1} \big|_{x=0} = k! (\lambda - H_0)^{-1} (V(\lambda - H_0)^{-1})^k$$

and

$$\frac{1}{k!} \frac{d^k}{dx^k} e^{it(H_0 + xV)} \big|_{x=0} = \frac{1}{2\pi i} \int_{\Gamma} e^{i\lambda t} (\lambda - H_0)^{-1} (V(\lambda - H_0)^{-1})^k d\lambda \quad (2.6.2)$$

Since $e^{it(H_0 + V)} = \frac{1}{2\pi i} \int_{\Gamma} e^{i\lambda t} (\lambda - H_0 - V)^{-1} d\lambda$ from (2.6.2) it follows

$$U_p(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{i\lambda t} \sum_{k=p}^{\infty} (\lambda - H_0)^{-1} (V(\lambda - H_0)^{-1})^k d\lambda = \frac{1}{2\pi i} \int_{\Gamma} e^{i\lambda t} G_p(\lambda) d\lambda$$

LEMMA 2.7 *Let $H_0 = H_0^*$ be an unbounded operator and $V = V^* \in C_p$. If $H_0^{(n)} = H_0 E(-n, n)$ (E is the spectral measure of H_0) and*

$$U_p^{(n)}(t) = e^{it(H_0^{(n)} + V)} - \sum_{k=0}^{p-1} \frac{1}{k!} \frac{d^k}{dx^k} e^{it(H_0^{(n)} + xV)} \big|_{x=0}$$

then for every $t \in \mathbb{R}$

$$\lim_{n \rightarrow \infty} \left| U_p(t) - U_p^{(n)}(t) \right|_1 = 0. \quad (2.7.1)$$

Proof. Since

$$U_p(t) = \frac{1}{(p-1)!} \int_0^1 m^{(p)}(x) (1-x)^{p-1} dx$$

and

$$U_p^{(n)}(t) = \frac{1}{(p-1)!} \int_0^1 m_n^{(p)}(x) (1-x)^{p-1} dx$$

where $m(x) = e^{it(H_0 + xV)}$ and $m_n(x) = e^{it(H_0^{(n)} + xV)}$, we obtain

$$\left| U_p(t) - U_p^{(n)}(t) \right|_1 \leq \frac{1}{(p-1)!} \int_0^1 \left| m^{(p)}(x) - m_n^{(p)}(x) \right|_1 (1-x)^{p-1} dx$$

From (2.1.1), (2.1.2) and [2, p. 119], Theorem 6.3 we have

$$\lim_{n \rightarrow \infty} \left| m^{(p)}(x) - m_n^{(p)}(x) \right|_1 = 0, \quad x \in (0, 1).$$

Now, since $\left| m^{(p)}(x) \right|_1 \leq |t|^p |V|_p^p$ and $\left| m_n^{(p)}(x) \right|_1 \leq |t|^p |V|_p^p$, (2.7.1) follows from the Lebesgue Dominated Convergence Theorem.

THEOREM 2.8 *If $V \in C_2$, $H_0 = H_0^*$ and $\varphi \in \mathcal{M}_2$, then*

- (1) $R_2 = \varphi(H_0 + V) - \varphi(H_0) - \frac{d}{dx} \varphi(H_0 + xV)|_{x=0} \in C_1$
- (2) *There exists a real function σ of bounded variation (σ depends only on H_0 and V) such that trace $R_2 = \int_R \varphi''(\lambda) d\sigma(\lambda)$*
- (3) $V_{-\infty}^\infty \sigma \leq |V|_2^2/2$
- (4) $\det_2 \left(I + V (H_0 - z)^{-1} \right) = \exp \left(- \int_R \frac{d\sigma(\lambda)}{(\lambda - z)^2} \right).$

Proof. (1) follows from Lemma 2.5. Let H_0 be a bounded operator, $\lambda_0 \in C \setminus R$ and $|\lambda_0| > 1 + \|H_0\| + \|V\|$. Now, by Runge's Theorem there exists a sequence of polynomials P_n such that $r_n(\lambda) := P_n(1/(\lambda - \lambda_0)) \rightrightarrows e^{i\lambda t}$ on $D = \{\lambda: |\lambda| \leq 1 + \|H_0\| + \|V\|\}$. Hence

$$r_n^{(\nu)}(\lambda) \rightrightarrows (it)^\nu e^{i\lambda t} \quad (\nu = 0, 1, 2, \dots) \quad \text{on } D. \quad (2.8.1)$$

Let $R_2^{(n)} = r_n(H_0 + V) - r_n(H_0) - \frac{d}{dx} r_n(H_0 + xV)|_{x=0}$. As in Lemma 2.6, we get

$$R_2^{(n)} = \frac{1}{2\pi i} \int_\Gamma r_n(\lambda) G_2(\lambda) d\lambda.$$

Now, by Lemma 2.6 we have

$$U_2(t) - R_2^{(n)}(t) = \frac{1}{2\pi i} \int_\Gamma (e^{i\lambda t} - r_n(\lambda)) G_2(\lambda) d\lambda$$

and

$$\left| U_2(t) - R_2^{(n)}(t) \right|_1 \leq \frac{1}{2\pi} \int_\Gamma |e^{i\lambda t} - r_n(\lambda)| \cdot \max_{\lambda \in \Gamma} |G_2(\lambda)|_1 \cdot |d\lambda| \longrightarrow 0 \quad (n \rightarrow \infty).$$

Hence $\lim_{n \rightarrow \infty} \text{trace } R_2^{(n)} = \text{trace } U_2(t)$. By Theorem 1, there exists a function σ of bounded variation (depending only on H_0 and V) such that $V_{-\infty}^\infty \sigma \leq |V|_2^2/2!$ and

$$\text{trace } R_2^{(n)} = \int_R r_n''(s) d\sigma(s) \quad (2.8.2)$$

From (2.8.1) and (2.8.2) it follows

$$\text{trace } U_2(t) = \int_R (it)^2 e^{its} d\sigma(s). \quad (2.8.3)$$

From (2.5.1) and (2.8.3) we conclude $\text{trace } R_2 = \int_R \varphi''(s) d\sigma(s)$.

Now consider the case when H_0 is not a bounded operator. Lemma 2.7 gives

$$\lim_{n \rightarrow \infty} \text{trace } U_2^{(n)}(t) = \text{trace } U_2(t). \quad (2.8.4)$$

From (2.8.3) it follows

$$\text{trace } U_2^{(n)}(t) = \int_R (it)^2 e^{its} d\sigma_n(s) \text{ and } V_{-\infty}^\infty \sigma_n \leq \frac{|V|_2^2}{2!}.$$

By (2.8.4) and the Helly election Theorem there exists a function σ of bounded variation ($V_{-\infty}^\infty \sigma \leq |V|_2^2/2!$) such that

$$\text{trace } U_2(t) = \int_R (it)^2 e^{its} d\sigma(s) \text{ and } \text{trace } R_2 = \int_R \varphi''(s) d\sigma(s).$$

The property (4) we obtain similarly as in [5].

THEOREM 2.9 *If $H_0 = H_0^* \in B(\mathcal{H})$, $V = V^* \in C_p$ ($p \geq 3$, $p \in \mathbb{N}$) and $\varphi \in \mathcal{M}_{p+1}$, then*

$$\text{trace } R_p = \frac{\text{trace } V^p}{p!} \varphi^{(p)}(0) + \int_R \varphi^{(p+1)}(x) \gamma(x) dx$$

where $\gamma \in L^2(R)$ is a function which depends only on V , H_0 and p .

Proof. From Lemma 2.6 it follows that $f(t) = \text{trace } U_p(t)$ is an entire function of the exponential type. On the other hand from (2.5.2) we get $|f(t)| \leq |t|^p |V|_p^p / p!$ for every $t \in \mathbb{R}$. Hence $f(0) = f'(0) = \dots = f^{(p-1)}(0) = 0$. From (2.6.1) we obtain

$$\lim_{t \rightarrow 0} \frac{f(t)}{(it)^p} = \frac{\text{trace } V^p}{p!}$$

So, $\frac{1}{t} \left(\frac{f(t)}{(it)^p} - \frac{\text{trace } V^p}{p!} \right) \in L^2(R)$ is an entire function of the exponential type. Now, by the Paley-Wiener Theorem we have

$$\frac{f(t)}{(it)^p} - \frac{\text{trace } V^p}{p!} = it \int_R e^{its} \gamma(s) ds$$

for some $\gamma \in L^2(R)$ and

$$f(t) = (it)^{p+1} \int_R e^{its} \gamma(s) ds + (it)^p \frac{\text{trace } V^p}{p!}. \quad (2.9.1)$$

The proof of Theorem 2.9 follows from (2.5.1) and (2.9.1).

COROLLARY 2.10. *If $H_0 = H_0^*$ is an unbounded operator, $V = V^* \in C_p$ ($p \geq 3$), then there exists a sequence $\gamma_n \in L^2(R)$ such that for every $\varphi \in \mathcal{M}_{p+1}$*

$$\text{trace } R_p = \frac{\text{trace } V^p}{p!} \varphi^{(p)}(0) + \lim_{n \rightarrow \infty} \int_R \varphi^{(p+1)}(x) \gamma_n(x) dx.$$

Proof. Since

$$\begin{aligned} R_p^{(n)} &= \varphi \left(H_0^{(n)} + V \right) - \sum_{k=0}^{p-1} \frac{1}{k!} \frac{d^k}{dx^k} \varphi \left(H_0^{(n)} + xV \right) \Big|_{x=0} \left(H_0^{(n)} = H_0 E(-n, n) \right) \\ &= \int_R g(t) U_p^{(n)}(t) dt, \end{aligned}$$

by Lemma 2.7 we get

$$\lim_{n \rightarrow \infty} \text{trace } R_p^{(n)} = \text{trace } R_p. \quad (2.10.1)$$

By Theorem 2.9 there exists a sequence $\gamma_n \in L^2(R)$ such that

$$\text{trace } R_p^{(n)} = \frac{\text{trace } V^p}{p!} \varphi^{(p)}(0) + \int_R \varphi^{(p+1)}(x) \gamma_n(x) dx$$

and the proof follows by (2.10.1).

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