

## TRACE FORMULAS FOR PERTURBATIONS OF OPERATORS WITH HILBERT-SCHMIDT RESOLVENTS

Bishnu Prasad Sedai

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**Abstract.** Trace formulas for self-adjoint perturbations  $V$  of self-adjoint operators  $H$  such that  $V$  is in Schatten class were obtained in the works of L.S. Koplienko, M.G. Krein, and the joint paper of D. Potapov, A. Skripka and F. Sukochev. In this article, we obtain an analogous trace formula under the assumptions that the perturbation  $V$  is bounded and the resolvent of  $H$  belongs to Hilbert-Schmidt class.

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### 1. INTRODUCTION

Let  $H$  be an unbounded self-adjoint operator,  $V$  a bounded self-adjoint operator on a separable Hilbert space  $\mathcal{H}$ ,  $f$  a sufficiently nice scalar function, and let  $f(H)$  and  $f(H + V)$  be defined by the functional calculus. Consider the remainder of the Taylor approximation

$$R_{n,H,V}(f) := f(H + V) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} \Big|_{t=0} f(H + tV),$$

where  $n \in \mathbb{N}$  and the Gâteaux derivatives  $\frac{d^k}{dt^k} \Big|_{t=0} f(H + tV)$  are evaluated in the uniform operator topology. If a perturbation  $V = V^*$  is in the Schatten-von Neumann ideal of compact operators  $\mathcal{S}^n$  (see, e.g., [6]), then the following trace formula holds (see [3–5])

$$\mathrm{Tr}(R_{n,H,V}(f)) = \int_{\mathbb{R}} f^{(n)}(t) \eta_n(t) dt, \quad (1.1)$$

where  $\eta_n = \eta_{n,H,V}$  is a real valued  $L^1$ -function depending only on  $H$  and  $V$ .

If the perturbations of the operators are not compact and no additional restriction on the initial operator  $H$  is imposed, then the trace  $\text{Tr}$  of  $R_{n,H,V}(f)$  is usually undefined. Noncompact perturbations mainly arise in the study of differential operators because they are multiplication by functions defined on  $\mathbb{R}^d$ , which are not compact operators. In this case, the condition that the perturbations are in some Schatten-von Neumann ideal of compact operators  $\mathcal{S}^n$  gets replaced by the restriction on the resolvent of the initial operators.

In this paper, we prove a trace formula similar to (1.1) under the different assumptions on  $H$ ,  $V$ , and  $f$ . We assume that the resolvent of  $H$  belongs to  $\mathcal{S}^2$ ,  $V = V^* \in \mathcal{B}(\mathcal{H})$  (where  $\mathcal{B}(\mathcal{H})$  is the algebra of bounded linear operators on  $\mathcal{H}$ ), and  $f \in C_c^n((a, b))$  (where  $C_c^n((a, b))$  is the space of  $n$  times continuously differentiable functions on  $\mathbb{R}$  that are compactly supported in  $(a, b) \subset \mathbb{R}$ ). We show that there exists a unique locally finite real-valued measure  $\mu_n = \mu_{n,H,V}$ ,  $n \geq 3$ , such that the following trace formula holds

$$\text{Tr}(R_{n,H,V}(f)) = \int_{\mathbb{R}} f^{(n)}(t) d\mu_n(t). \tag{1.2}$$

Similar formula for  $n = 1$  and  $n = 2$  but with the absolutely continuous measure  $\mu_n$  was established in [1] and [7], respectively. The formula obtained in those cases holds for  $f \in C_c^{n+1}(\mathbb{R})$  whereas, the formula (1.2) can also be applied to  $f \in C_c^n(\mathbb{R})$ .

We prove the result following delicate methods of noncommutative analysis developed in [7]. We first show that  $R_{n-1,H,V}(f)$  and  $\frac{d^{n-1}}{dt^{n-1}} \Big|_{t=0} f(H + tV)$  are both trace class operators and prove the estimate

$$|\text{Tr}(R_{n,H,V}(f))| \leq C_{n,a,b,H,V} \cdot \|f^{(n)}\|_{L^\infty([a,b])},$$

where  $C_{n,a,b,H,V}$  is a constant depending on  $n$ ,  $a$ ,  $b$ ,  $H$ , and  $V$ . Then, we use the Riesz representation theorem for a functional in  $(C_c(\mathbb{R}))^*$  to find a unique locally finite real-valued measure  $\mu_n$  that satisfies (1.2).

We divide this paper into two sections. In the first section, we provide preliminaries on operator derivatives and its trace norm estimates. In the second section, we prove the main result.

## 2. PRELIMINARIES

We start the section with the following useful estimate for the resolvent operators and which follows from the functional calculus of self-adjoint operators.

**Lemma 2.1** ([2, Appendix B, Lemma 6]). *Let  $H = H^*$  be defined in  $\mathcal{H}$  and  $W = W^* \in \mathcal{B}(\mathcal{H})$ , then*

$$(I + (H + W)^2)^{-1} \leq (I + \|W\| + \|W\|^2)(I + H^2)^{-1}.$$

The following is a definition of the Gâteaux derivative of operator functions.

**Definition 2.2.** Let  $H$  be a self-adjoint (unbounded) operator in  $\mathcal{H}$  and  $V = V^* \in \mathcal{B}(\mathcal{H})$ . Let  $f : \mathbb{R} \mapsto \mathbb{C}$  be a bounded function. Then, the Gâteaux derivative of the mapping  $H \rightarrow f(H)$  at  $H$  in the direction  $V$  is defined by

$$\left. \frac{d}{ds} \right|_{s=0} f(H + sV) = \lim_{s \rightarrow 0} \frac{f(H + sV) - f(H)}{s},$$

if the limit exists in the operator norm (uniform operator topology).

We need the following integral representation for the  $n$ th order Taylor remainder.

**Lemma 2.3** ([7, Theorem 2.7]). *Let  $H = H^*$  be defined in  $\mathcal{H}$  and  $V = V^* \in \mathcal{B}(\mathcal{H})$ . If  $f \in C_c^{n+1}(\mathbb{R})$ , then*

$$R_{n,H,V}(f) = \frac{1}{(n-1)!} \int_0^1 (1-t)^{n-1} \left. \frac{d^n}{ds^n} \right|_{s=t} f(H + sV) dt,$$

where the integral is defined for every  $y \in \mathcal{H}$  by

$$\left( \int_0^1 (1-t)^{n-1} \left. \frac{d^n}{ds^n} \right|_{s=t} f(H + sV) dt \right) y = \int_0^1 (1-t)^{n-1} \left. \frac{d^n}{ds^n} \right|_{s=t} f(H + sV) y dt.$$

Under the assumption  $(I + H^2)^{-1/2} \in \mathcal{S}^2$ , we have the following trace norm estimate for the  $n$ th order Gâteaux derivative.

**Lemma 2.4** ([7, Lemma 3.6]). *Let  $H = H^*$  satisfy  $(I + H^2)^{-1/2} \in \mathcal{S}^2$  and let  $V = V^* \in \mathcal{B}(\mathcal{H})$ . Denote  $u(t) = (1 + t^2)^{1/2}$ . Then, for every  $n \in \mathbb{N}$  and  $f \in C_c^{n+1}(\mathbb{R})$ ,  $\frac{1}{n!} \cdot \left. \frac{d^n}{dt^n} \right|_{t=0} f(H + tV) \in \mathcal{S}^1$  and*

$$\left\| \frac{1}{n!} \cdot \left. \frac{d^n}{dt^n} \right|_{t=0} f(H + tV) \right\|_1 \leq C_{f,n} \cdot \|(I + H^2)^{-1/2}\|_2^2 \cdot \|V\|^n,$$

where

$$C_{f,1} \leq \sqrt{2} \left( \|(fu^2)'\|_2 + \|(fu^2)''\|_2 \right) + 2\|fu^2\|_\infty \quad (2.1)$$

and for  $n \geq 2$ ,

$$\begin{aligned} C_{f,n} &\leq \frac{\sqrt{2}}{n!} \left( \|(fu^2)^{(n)}\|_2 + \|(fu^2)^{(n+1)}\|_2 \right) \\ &\quad + \frac{n(n+3)}{2} \cdot \max_{1 \leq k \leq n} \left\{ \|f\|_\infty, \|fu\|_\infty, \frac{\sqrt{2}}{k!} \left( \|f^{(k)}\|_2 + \|f^{(k+1)}\|_2 \right) \right\}, \\ &\quad \frac{\sqrt{2}}{k!} \left( \|(fu)^{(k)}\|_2 + \|(fu)^{(k+1)}\|_2 \right) \} \\ &\quad \times \text{const} \cdot \max_{2 \leq j \leq n} \left( \|u^{(j)}\|_2 + \|u^{(j+1)}\|_2 \right)^2. \end{aligned} \quad (2.2)$$

Using Lemmas 2.1 and 2.4, we have the following lemma.

**Lemma 2.5.** *Let  $H = H^*$  satisfy  $(I + H^2)^{-1/2} \in \mathcal{S}^2$  and let  $V = V^* \in \mathcal{B}(\mathcal{H})$ . Denote  $u(t) = (1 + t^2)^{1/2}$ . Then, for every  $n \in \mathbb{N}$  and  $f \in C_c^{n+1}(\mathbb{R})$ ,  $\frac{1}{n!} \cdot \frac{d^n}{ds^n} \Big|_{s=t} f(H + sV) \in \mathcal{S}^1$  and for all  $t \in (0, 1)$*

$$\left\| \frac{1}{n!} \cdot \frac{d^n}{ds^n} \Big|_{s=t} f(H + sV) \right\|_1 \leq C_{f,n} \cdot \|(I + H^2)^{-1/2}\|_2^2 \cdot (\|V\|^n + \|V\|^{n+1} + \|V\|^{n+2}),$$

where  $C_{f,n}$  satisfies (2.1) for  $n = 1$  and (2.2) for  $n \geq 2$ .

*Proof.* From Definition 2.2, it follows that

$$\frac{d}{ds} \Big|_{s=t} f(H + sV) = \frac{d}{ds} \Big|_{s=0} f(H + (s + t)V).$$

Now using Lemma 2.4, we have  $\frac{1}{n!} \cdot \frac{d^n}{ds^n} \Big|_{s=t} f(H + sV) \in \mathcal{S}^1$  and

$$\begin{aligned} \left\| \frac{1}{n!} \cdot \frac{d^n}{ds^n} \Big|_{s=t} f(H + sV) \right\|_1 &\leq C_{f,n} \cdot \|(I + (H + tV)^2)^{-1/2}\|_2^2 \cdot \|V\|^n \\ &\leq C_{f,n} \cdot \|(I + H^2)^{-1/2}\|_2^2 \cdot (\|V\|^n + \|V\|^{n+1} + \|V\|^{n+2}), \end{aligned}$$

where the last inequality follows from Lemma 2.1 and the fact that  $t \in (0, 1)$ . □

We estimate the constant  $C_{f,n}$  in terms of the supremum norm of  $(n + 1)$ th derivative of  $f$ .

**Lemma 2.6.** *Let  $f \in C_c^{n+1}((a, b))$ ,  $n \in \mathbb{N}$ , and  $u(t) = (1 + t^2)^{1/2}$ . If  $C_{a,b,f,n}$  satisfies (2.1) for  $n = 1$  and (2.2) for  $n \geq 2$ , then*

$$C_{a,b,f,n} \leq \|f^{(n+1)}\|_{L^\infty([a,b])} \cdot C_{a,b,n}, \quad n \in \mathbb{N}, \tag{2.3}$$

where

$$C_{a,b,1} = 24 \cdot \max\{1, (b - a)^2\} \cdot \max\left\{2, \|u^2\|_{L^\infty([a,b])}, \|(u^2)'\|_{L^\infty([a,b])}\right\} \tag{2.4}$$

and for  $n \geq 2$ ,

$$\begin{aligned} C_{a,b,n} &= \left[ \frac{4(b - a)^{1/2}}{n!} + \frac{n(n + 3)}{2} \cdot \max\{1, 4(b - a)^{1/2}\} \right. \\ &\quad \times \text{const} \cdot \max_{2 \leq j \leq n} \left( \|u^{(j)}\|_{L^2([a,b])} + \|u^{(j+1)}\|_{L^2([a,b])} \right)^2 \left. \right] \cdot 2^n \cdot \max\{1, (b - a)^{n+1}\} \\ &\quad \times \max_{0 \leq k \leq n+1} \left\{ 2, \|u^2\|_{L^\infty([a,b])}, \|(u^2)'\|_{L^\infty([a,b])}, \|u^{(k)}\|_{L^\infty([a,b])} \right\}. \end{aligned} \tag{2.5}$$

*Proof.* We prove the case  $n \geq 2$ . The case  $n = 1$  is similar to that of  $n \geq 2$  and, hence, omitted. Here, we denote  $\|\cdot\|_2 = \|\cdot\|_{L^2([a,b])}$  and  $\|\cdot\|_\infty = \|\cdot\|_{L^\infty([a,b])}$ . For  $f \in C_c^{n+1}((a,b))$ ,

$$\|f^{(j)}\|_2 \leq \|f^{(j)}\|_\infty \cdot (b-a)^{1/2}, \quad 0 \leq j \leq n+1. \quad (2.6)$$

Using (2.6), we obtain

$$\begin{aligned} & C_{a,b,f,n} \\ & \leq \frac{\sqrt{2}}{n!} \left( \|(fu^2)^{(n)}\|_\infty (b-a)^{1/2} + \|(fu^2)^{(n+1)}\|_\infty (b-a)^{1/2} \right) \\ & \quad + \frac{n(n+3)}{2} \cdot \max_{1 \leq k \leq n} \left\{ \|f\|_\infty, \|fu\|_\infty, \frac{\sqrt{2}}{k!} \left( \|f^{(k)}\|_\infty (b-a)^{1/2} + \|f^{(k+1)}\|_\infty (b-a)^{1/2} \right), \right. \\ & \quad \left. \frac{\sqrt{2}}{k!} \left( \|(fu)^{(k)}\|_\infty (b-a)^{1/2} + \|(fu)^{(k+1)}\|_\infty (b-a)^{1/2} \right) \right\} \\ & \quad \times \text{const} \cdot \max_{2 \leq j \leq n} \left( \|u^{(j)}\|_2 + \|u^{(j+1)}\|_2 \right)^2. \end{aligned} \quad (2.7)$$

Since

$$\begin{aligned} \|(fg)^{(k)}\|_\infty &= \left\| \sum_{j=0}^k \binom{k}{j} f^{(j)} g^{(k-j)} \right\|_\infty \leq \sum_{j=0}^k \binom{k}{j} \|f^{(j)}\|_\infty \|g^{(k-j)}\|_\infty \\ &\leq 2^k \cdot \max_{0 \leq j \leq k} \|f^{(j)}\|_\infty \cdot \max_{0 \leq l \leq k} \|g^{(l)}\|_\infty, \end{aligned}$$

for  $0 \leq i \leq n+1$ , we have

$$\begin{aligned} \|(fu^2)^{(i)}\|_\infty &\leq 2^i \cdot \max_{0 \leq j \leq i} \|f^{(j)}\|_\infty \cdot \max_{0 \leq l \leq i} \|(u^2)^{(l)}\|_\infty \\ &\leq 2^{n+1} \cdot \max \left\{ \|f\|_\infty, \|f'\|_\infty, \dots, \|f^{(n+1)}\|_\infty \right\} \\ &\quad \times \max \left\{ \|u^2\|_\infty, \|(u^2)'\|_\infty, \dots, \|(u^2)^{(n+1)}\|_\infty \right\}. \end{aligned} \quad (2.8)$$

Since, for  $f \in C_c^{n+1}((a,b))$ ,

$$\|f^{(j)}\|_\infty \leq \|f^{(n+1)}\|_\infty \cdot (b-a)^{n+1-j}, \quad 0 \leq j \leq n+1,$$

(2.8) is bounded by

$$\begin{aligned} \|(fu^2)^{(i)}\|_\infty &\leq 2^{n+1} \cdot \|f^{(n+1)}\|_\infty \cdot \max \left\{ (b-a)^{n+1}, (b-a)^n, \dots, 1 \right\} \\ &\quad \times \max \left\{ \|u^2\|_\infty, \|(u^2)'\|_\infty, \dots, \|(u^2)^{(n+1)}\|_\infty \right\}, \end{aligned} \quad (2.9)$$

for  $0 \leq i \leq n + 1$ . Since  $\max_{1 \leq i \leq n+1} \{1, (b - a)^i\} \leq \max\{1, (b - a)^{n+1}\}$ ,  $(u^2)'' \equiv 2$ , and  $(u^2)^{(n+1)} = 0$ , for  $n \geq 2$ , (2.9) is bounded by

$$\begin{aligned} \|(fu^2)^{(i)}\|_\infty &\leq 2^{n+1} \cdot \|f^{(n+1)}\|_\infty \cdot \max\{1, (b - a)^{n+1}\} \cdot \max\{2, \|u^2\|_\infty, \|(u^2)'\|_\infty\} \\ &\leq 2^{n+1} \cdot \|f^{(n+1)}\|_\infty \cdot \max\{1, (b - a)^{n+1}\} \\ &\quad \times \max_{0 \leq k \leq n+1} \{2, \|u^2\|_\infty, \|(u^2)'\|_\infty, \|u^{(k)}\|_\infty\}, \quad 0 \leq i \leq n + 1. \end{aligned} \tag{2.10}$$

Similarly, for  $0 \leq i \leq n + 1$ , we have

$$\begin{aligned} \|f^{(i)}\|_\infty &\leq 2^{n+1} \cdot \|f^{(n+1)}\|_\infty \cdot \max\{1, (b - a)^{n+1}\} \\ &\quad \times \max_{0 \leq k \leq n+1} \{2, \|u^2\|_\infty, \|(u^2)'\|_\infty, \|u^{(k)}\|_\infty\}, \end{aligned} \tag{2.11}$$

and

$$\begin{aligned} \|(fu)^{(i)}\|_\infty &\leq 2^{n+1} \cdot \|f^{(n+1)}\|_\infty \cdot \max\{1, (b - a)^{n+1}\} \\ &\quad \times \max_{0 \leq k \leq n+1} \{2, \|u^2\|_\infty, \|(u^2)'\|_\infty, \|u^{(k)}\|_\infty\}. \end{aligned} \tag{2.12}$$

Using (2.10)–(2.12), we obtain that

$$\begin{aligned} C_{a,b,f,n} &\leq \|f^{(n+1)}\|_\infty \cdot \left[ \frac{2^{3/2}(b - a)^{1/2}}{n!} + \frac{n(n + 3)}{2} \cdot \max\{1, 2^{3/2}(b - a)^{1/2}\} \right] \\ &\quad \times \text{const} \cdot \max_{2 \leq j \leq n} \left( \|u^{(j)}\|_2 + \|u^{(j+1)}\|_2 \right)^2 \cdot 2^n \cdot \max\{1, (b - a)^{n+1}\} \\ &\quad \times \max_{0 \leq k \leq n+1} \{2, \|u^2\|_\infty, \|(u^2)'\|_\infty, \|u^{(k)}\|_\infty\} \\ &\leq \|f^{(n+1)}\|_\infty \cdot \left[ \frac{4(b - a)^{1/2}}{n!} + \frac{n(n + 3)}{2} \cdot \max\{1, 4(b - a)^{1/2}\} \right] \\ &\quad \times \text{const} \cdot \max_{2 \leq j \leq n} \left( \|u^{(j)}\|_2 + \|u^{(j+1)}\|_2 \right)^2 \cdot 2^n \cdot \max\{1, (b - a)^{n+1}\} \\ &\quad \times \max_{0 \leq k \leq n+1} \{2, \|u^2\|_\infty, \|(u^2)'\|_\infty, \|u^{(k)}\|_\infty\} \\ &= \|f^{(n+1)}\|_\infty \cdot C_{a,b,n}, \quad n \geq 2, \end{aligned}$$

where  $C_{a,b,n}$  is given by (2.5). □

### 3. MAIN SECTION

Now we are in a position to prove the main result.

**Theorem 3.1.** *Let  $H = H^*$  satisfy  $(I + H^2)^{-1/2} \in \mathcal{S}^2$  and let  $V = V^* \in \mathcal{B}(\mathcal{H})$ . Then, there is a unique locally finite real-valued measure  $\mu_n = \mu_{n,H,V}$ ,  $n \geq 3$ , with total variation on the segment  $[a, b]$ ,  $a, b \in \mathbb{R}$*

$$\int_{[a,b]} d|\mu_n| \leq 4 \cdot C_{a,b,n-1} \cdot \|(I + H^2)^{-1}\|_1 \cdot \max_{n-1 \leq k \leq n+1} \|V\|^k, \quad (3.1)$$

where  $C_{a,b,k}$ ,  $k \geq 2$ , is given by (2.5) such that

$$\mathrm{Tr}(R_{n,H,V}(f)) = \int_{\mathbb{R}} f^{(n)}(\lambda) d\mu_n(\lambda),$$

for  $f \in C_c^n((a, b))$ .

*Proof.* By Lemmas 2.5 and 2.3, we have  $R_{n-1,H,V}(f) \in \mathcal{S}^1$  and

$$\left| \mathrm{Tr}(R_{n-1,H,V}(f)) \right| \leq C_{a,b,f,n-1} \cdot \|(I + H^2)^{-1/2}\|_2^2 \cdot (\|V\|^{n-1} + \|V\|^n + \|V\|^{n+1}), \quad (3.2)$$

where  $C_{a,b,f,k}$  satisfies (2.2) for  $k \geq 2$ . By Lemma 2.6 and the fact that

$$\|(I + H^2)^{-1/2}\|_2^2 = \|(I + H^2)^{-1}\|_1,$$

the inequality (3.2) is bounded by

$$\begin{aligned} & \left| \mathrm{Tr}(R_{n-1,H,V}(f)) \right| \\ & \leq \|f^{(n)}\|_{L^\infty([a,b])} \cdot C_{a,b,n-1} \cdot \|(I + H^2)^{-1}\|_1 \cdot (\|V\|^{n-1} + \|V\|^n + \|V\|^{n+1}). \end{aligned} \quad (3.3)$$

Similarly, by Lemmas 2.4 and 2.6, we have  $\frac{1}{(n-1)!} \cdot \frac{d^{n-1}}{dt^{n-1}} \Big|_{t=0} f(H + tV) \in \mathcal{S}^1$  and

$$\begin{aligned} & \left| \mathrm{Tr} \left( \frac{1}{(n-1)!} \cdot \frac{d^{n-1}}{dt^{n-1}} \Big|_{t=0} f(H + tV) \right) \right| \\ & \leq \|f^{(n)}\|_{L^\infty([a,b])} \cdot C_{a,b,n-1} \cdot \|(I + H^2)^{-1}\|_1 \cdot \|V\|^{n-1}. \end{aligned} \quad (3.4)$$

Combining (3.3) and (3.4), we get

$$\left| \mathrm{Tr}(R_{n,H,V}(f)) \right| \leq \|f^{(n)}\|_{L^\infty([a,b])} \cdot 4 \cdot C_{a,b,n-1} \cdot \|(I + H^2)^{-1}\|_1 \cdot \max_{n-1 \leq k \leq n+1} \|V\|^k.$$

Hence, by the Riesz representation theorem for a functional in  $(C_c(\mathbb{R}))^*$ , there is a unique locally finite real-valued measure  $\mu_n = \mu_{n,H,V}$ ,  $n \geq 3$ , with total variation on the segment  $[a, b]$  satisfying (3.1) such that

$$\mathrm{Tr}(R_{n,H,V}(f)) = \int_{\mathbb{R}} f^{(n)}(\lambda) d\mu_n(\lambda). \quad \square$$

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Bishnu Prasad Sedai  
bishnus7@vt.edu

Department of Mathematics  
Virginia Polytechnic Institute and State University  
225 Stanger Street, Blacksburg, VA 24061, USA

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