

# Two Variable Trace Formula

Kalyan B. Sinha

J.N.Centre for Advanced Scientific Research  
and  
Indian Institute of Science, Bangalore, India.

(in collaboration with Arup Chattopadhyay)

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# Notations

- $\mathcal{H} \equiv$  Separable Hilbert space
- $\mathcal{B}(\mathcal{H}) \equiv$  Set of bounded operators
- $\mathcal{B}_1(\mathcal{H}) \equiv$  Set of trace class operators
- $\mathcal{B}_2(\mathcal{H}) \equiv$  Set of Hilbert-Schmidt class operators
- $\mathcal{B}_p(\mathcal{H}) \equiv$  Schatten-p class operators
- $\|\cdot\|_p \equiv$  Schatten-p norm
- $\mathcal{P}([a, b]) \equiv$  Set of polynomials with complex coefficients on  $[a, b]$
- $C([a, b]) \equiv$  Set of continuous functions on  $[a, b]$
- $\sigma(H) \equiv$  Spectrum of the operator  $H$

# Introduction

- Let  $H$  and  $H_0$  be two possibly unbounded self-adjoint operators in a separable Hilbert space  $\mathcal{H}$  such that  $V = H - H_0 \in \mathcal{B}_1(\mathcal{H})$ . Then Krein proved that there exists a unique real-valued  $L^1(\mathbb{R})$ -function  $\xi$  with support in the interval  $[a, b]$  such that

$$\text{Tr}[\phi(H_0 + V) - \phi(H_0)] = \int_a^b \phi'(\lambda) \xi(\lambda) d\lambda, \quad (1)$$

for a large class of functions  $\phi$  (where  $a = \min\{\inf \sigma(H), \inf \sigma(H_0)\}$  and  $b = \max\{\sup \sigma(H), \sup \sigma(H_0)\}$ ).

- The function  $\xi$  is known as Krein's spectral shift function and the relation (1) is called Krein's trace formula.
- The original proof of Krein [4] uses analytic function theory.
- Later, Voiculescu approached the trace formula (1) from a different direction.

# Introduction

- If  $H$  and  $H_0$  are bounded, then Voiculescu [6] proved that

$$\mathrm{Tr} [p(H) - p(H_0)] = \lim_{n \rightarrow \infty} \mathrm{Tr} [p(H_n) - p(H_{0,n})], \quad (2)$$

where  $p$  is a polynomial and  $H_n, H_{0,n}$  are finite-dimensional approximation of  $H$  and  $H_0$  respectively (constructed by adapting Weyl-von Neumann theorem).

- Then one constructs the spectral shift function in the finite dimensional case and finally the formula is extended to the infinite dimensional case.
- Later Sinha and Mohapatra [5] used a similar method to get the same result for the unbounded self-adjoint case.
- More recently, Potapov, Skripka and Sukochev [2] has proven the trace-formula for all orders, obtaining a kind of Taylor's theorem under trace.

# Introduction

- It is natural to ask similar questions for a pair of commuting self-adjoint  $n$ -tuples, particularly an appropriate adaptation of Krein's formula (1) to two and higher dimensions.
- Here our aim is to formulate a relevant question for a pair of commuting bounded self-adjoint tuples and use finite-dimensional approximation to get a trace formula.
- Before going to the main result in this talk first we start with an approximation result which we have adapted from the proof of Weyl-von Neumann-Berg Theorem.

# Approximation Results

- A result due to Weyl and von Neumann [3] proves that for a self-adjoint operator  $A$  that given  $\epsilon > 0$ ,  $\exists K \in \mathcal{B}_2(\mathcal{H})$  such that  $\|K\|_2 < \epsilon$  and  $A + K$  has pure point spectrum.
- Later Berg extended this to an  $n$ -tuples of bounded commuting self-adjoint operators  $(A_1, A_2, \dots, A_n)$ , which says that given  $\epsilon > 0$ ,  $\exists \{K_j\}_{j=1}^n$  of compact operators such that  $\|K_j\| < \epsilon \forall j$  and  $\{A_j - K_j\}_{j=1}^n$  is a commuting family of bounded self-adjoint operators with pure point spectra.
- Here we extend in the next theorem the ideas of the proof of Berg's result as given in [1].
- It is worth mentioning that Voiculescu [7] had earlier obtained related (though not the same) results.

# Approximation Results

## Theorem 1

Let  $\{A_i\}_{1 \leq i \leq n}$  be a commuting family of bounded self-adjoint operators in an infinite-dimensional separable Hilbert space  $\mathcal{H}$ . Then there exists a sequence  $\{P_N\}$  of finite-rank projections such that  $\{P_N\} \uparrow I$  as  $N \rightarrow \infty$  and such that there exists a commuting family of bounded self-adjoint operators  $\{B_i^{(N)}\}_{1 \leq i \leq n}$  with the properties that for  $p \geq n$  and for each  $i$  ( $1 \leq i \leq n$ ), as  $N \rightarrow \infty$ ,

$$(i) P_N B_i^{(N)} P_N = B_i^{(N)} P_N, \quad (ii) \left\| A_i - B_i^{(N)} \right\|_p \rightarrow 0,$$

$$(iii) \left\| [A_i, P_N] \right\|_p \rightarrow 0,$$

$$(iv) \left\| P_N A_i P_N - B_i^{(N)} P_N \right\|_p \rightarrow 0 \quad \text{and} \quad (v) \{B_i^{(N)} P_N\} \uparrow A_i.$$



## Sketch of the Proof of Theorem 1:

- Without loss of generality we assume that  $0 \leq A_i \leq I$  for all  $1 \leq i \leq n$ , and we start with the representation for each  $i$ ,

$$A_i = \sum_{k=1}^{\infty} 2^{-k} E_k^{(i)},$$

where  $E_k^{(i)} = E_{A_i} \left( \bigcup_{j=1}^{2^{k-1}} (2^{-k}(2j-1), 2^{-k}(2j)] \right)$  with  $E_{A_i}$  the spectral measure associated to the bounded self-adjoint operator  $A_i$ .

- Next set for  $N \in \mathbb{N}$  (the set of natural numbers),

$$\mathcal{L}_N \equiv \text{span} \left\{ \left[ \prod_{k=1}^N \prod_{i=1}^n \left( E_k^{(i)} \right)^{\epsilon} \right] f_j \mid 1 \leq j \leq N; \epsilon = \pm 1 \right\},$$

where  $\{f_1, f_2, \dots, f_N, \dots\}$  be a countable orthonormal basis of  $\mathcal{H}$  and  $\left( E_k^{(i)} \right)^1 = E_k^{(i)}$  and  $\left( E_k^{(i)} \right)^{-1} = I - E_k^{(i)}$ .

- Then  $\mathcal{L}_N$  is a finite dimensional subspace of  $\mathcal{H}$  and it has the following properties:

$$(a) \quad \mathcal{L}_N \subseteq \mathcal{L}_{N+1}, \quad (b) \quad \overline{\left( \bigcup_{N=1}^{\infty} \mathcal{L}_N \right)} = \mathcal{H},$$

$$(c) \quad \dim(\mathcal{L}_N) \leq N(2^n - 1)^N + N.$$

- Set  $P_N$  to be the finite rank projection associated with the finite dimensional subspace  $\mathcal{L}_N$  and observe that  $\{P_N\}$  increases to  $I$ .
- Next define

$$B_i^{(N)} = \sum_{k=1}^N 2^{-k} E_k^{(i)} + \sum_{k=N+1}^{\infty} 2^{-k} E_k^{(i)} (I - P_k).$$

- Then  $\{B_i^{(N)}\}_{1 \leq i \leq n}$  is a commuting family of bounded self-adjoint operators.

- Furthermore,  $A_i - B_i^{(N)} = \sum_{k=N+1}^{\infty} 2^{-k} E_k^{(i)} P_k$  and

$$\begin{aligned} \left\| A_i - B_i^{(N)} \right\|_n &\leq \sum_{k=N+1}^{\infty} 2^{-k} \|P_k\|_n \leq \sum_{k=N+1}^{\infty} 2^{-k} \left[ k \{1 + (2^n - 1)^k\} \right]^{\frac{1}{n}} \\ &= \sum_{k=N+1}^{\infty} k^{\frac{1}{n}} \left[ 2^{-nk} + (1 - 2^{-n})^k \right]^{\frac{1}{n}} \\ &\leq \sum_{k=N+1}^{\infty} k^{\frac{1}{n}} 2^{-k} + \sum_{k=N+1}^{\infty} k^{\frac{1}{n}} \left[ (1 - 2^{-n})^{\frac{1}{n}} \right]^k, \end{aligned}$$

where we have used that for  $a, b > 0$ ,  $(a + b)^{\frac{1}{n}} \leq (a^{\frac{1}{n}} + b^{\frac{1}{n}})$ .

- Since for fixed  $n$ ,  $(1 - 2^{-n})^{\frac{1}{n}} < 1$ , and since  $\sum_{k=1}^{\infty} k^{\frac{1}{n}} \alpha^k < \infty$  for  $\alpha < 1$ , it follows from the above that for each  $i$  ( $1 \leq i \leq n$ ) and any  $p \geq n$ ,

$$\left\| A_i - B_i^{(N)} \right\|_p \leq 2^{\left(1 - \frac{n}{p}\right)} \left\| A_i - B_i^{(N)} \right\|_n^{\frac{n}{p}} \rightarrow 0 \quad \text{as } N \rightarrow \infty. \square$$

## Remark

The choice that  $0 \leq A_i \leq I$  does not materially affect the calculations of the above theorem. For if  $C_i \in \mathcal{B}(\mathcal{H})$  ( $1 \leq i \leq n$ ), then we can set

$$A_i = (2\|C_i\|)^{-1} C_i + \frac{1}{2}I$$

so that  $0 \leq A_i \leq I$  and thus  $C_i = 2\|C_i\|(\sum 2^{-k} E_k^{(i)} - \frac{1}{2}I)$ . Thus choosing

$$B_i^{(N)} = 2\|C_i\| \left\{ \sum_{k=1}^N 2^{-k} E_k^{(i)} + \sum_{k=N+1}^{\infty} (I - P_k) E_k^{(i)} - \frac{1}{2}I \right\}$$

one has  $\|[C_i, B_i^{(N)}]\|_p = 2\|C_i\| \|[A_i, B_i^{(N)}]\|_p \rightarrow 0$  as  $N \rightarrow \infty$  for  $p \geq n$ .

# Trace Formula in Finite Dimension

## Theorem 2

Let  $P$  and  $Q$  be two finite-dimensional projections in a (infinite dimensional separable) Hilbert space  $\mathcal{H}$ . Assume furthermore the two commuting pairs of bounded self-adjoint operator tuples  $(H_1^0, H_2^0)$  and  $(H_1, H_2)$  are acting in the common reducing subspaces  $P\mathcal{H}$  and  $Q\mathcal{H}$  respectively. Also let  $\sigma(H_1), \sigma(H_2), \sigma(H_1^0), \sigma(H_2^0)$  be in  $[a, b]$  and let  $\phi, \psi$  be in  $C^1([a, b])$ . Then

$$\begin{aligned} & \operatorname{Tr} \left\{ Q \left( \phi(H_1) - \phi(H_1^0) \right) P \left( \psi(H_2) - \psi(H_2^0) \right) Q \right\} \\ &= \int_{[a,b]^2} \phi'(x) \psi'(y) \xi(x, y) \, dx dy, \end{aligned} \quad (3)$$

where  $\xi(x, y) = \operatorname{Tr} \left\{ Q \left[ E_{H_1}(x) - E_{H_1^0}(x) \right] P \left[ E_{H_2}(y) - E_{H_2^0}(y) \right] Q \right\}$  and  $E_{H_1}(\cdot), E_{H_2}(\cdot), E_{H_1^0}(\cdot), E_{H_2^0}(\cdot)$  are the spectral measures of the operators  $H_1, H_2, H_1^0, H_2^0$  respectively.

## Sketch of the Proof of Theorem 2:

By the spectral theorem of self-adjoint operators, Fubini's theorem and performing integration by-parts appropriately we can prove the above theorem.  $\square$

- In the next theorem we gave an equivalent description of the expression on the left hand side of the equation (3), in terms of divided differences and a  $\mathcal{B}_2(\mathcal{H})$ -valued spectral measure.

# Trace Formula in Finite Dimension

## Theorem 3

Under the hypotheses of Theorem 2,

$$\mathrm{Tr}\left\{Q\left(\phi(H_1) - \phi(H_1^0)\right)P\left(\psi(H_2) - \psi(H_2^0)\right)Q\right\}$$

$$= \int_{[a,b]^2} \int_{[a,b]^2} \left\{ \frac{\phi(x_1) - \phi(x_2)}{x_1 - x_2} \right\} \left\{ \frac{\psi(y_1) - \psi(y_2)}{y_1 - y_2} \right\} \bullet$$

$$\left\langle \left( H_1 - H_1^0 \right), PE_{\underline{H}^0}(dx_2 \times dy_1) \left( H_2 - H_2^0 \right) E_{\underline{H}}(dx_1 \times dy_2) Q \right\rangle_2,$$

where we have written  $\underline{H}^0 = (H_1^0, H_2^0)$ ,  $\underline{H} = (H_1, H_2)$ ;  $E_{\underline{H}^0}(\cdot)$  and  $E_{\underline{H}}(\cdot)$  are the associated spectral measures of the operators tuples  $\underline{H}^0$  and  $\underline{H}$  respectively on the Borel sets of  $[a, b]^2$ , and where  $\langle \cdot, \cdot \rangle_2$  denotes the inner product of the Hilbert space  $\mathcal{B}_2(\mathcal{H})$ .

- Note that the above theorem (Theorem 3) can also be extended in an infinite dimensional setting.

### Sketch of the Proof of Theorem 3:

In  $\mathcal{H}$ , using the ideas of double spectral integrals, trace properties, Fubini's theorem and the fact that  $(H_1^0, H_2^0)$ ,  $(H_1, H_2)$  are two commuting pairs of self-adjoint operators, we can prove the above theorem.  $\square$



# Main Theorem

## Theorem 4

Let  $(H_1^0, H_2^0)$  and  $(H_1, H_2)$  be two commuting pairs of bounded self-adjoint operators in a separable Hilbert space  $\mathcal{H}$  such that  $H_j - H_j^0 \equiv V_j \in \mathcal{B}_2(\mathcal{H})$  and such that  $\sigma(H_j), \sigma(H_j^0) \subseteq [a, b]$  for  $j = 1, 2$ . Then there exists a unique complex Borel measure  $\mu$  on  $[a, b]^2$  such that

$$\mathrm{Tr} \left\{ \left( \phi(H_1) - \phi(H_1^0) \right) \left( \psi(H_2) - \psi(H_2^0) \right) \right\} = \int_{[a,b]^2} \phi'(x) \psi'(y) \mu(dx \times dy),$$

where  $\phi, \psi \in \mathcal{P}([a, b])$ .

## Sketch of the Proof of Theorem 4:

- **(Finite Dimensional Reduction):**

Applying approximation results (Theorem 1) to the pairs  $(H_1^0, H_2^0)$  and  $(H_1, H_2)$  we get two commuting pairs of finite dimensional self-adjoint operators  $(H_1^{0(N)}, H_2^{0(N)})$  and  $(H_1^{(N)}, H_2^{(N)})$  in  $P_N^0 \mathcal{H}$  and  $P_N \mathcal{H}$  respectively, such that

$$\| [H_j^0, P_N^0] \|_p, \quad \left\| P_N^0 H_j^0 P_N^0 - H_j^{0(N)} P_N^0 \right\|_p \longrightarrow 0 \text{ as } N \longrightarrow \infty \text{ for } p \geq 2, j = 1, 2,$$

and

$$\| [H_j, P_N] \|_p, \quad \left\| P_N H_j P_N - H_j^{(N)} P_N \right\|_p \longrightarrow 0 \text{ as } N \longrightarrow \infty \text{ for } p \geq 2, j = 1, 2,$$

where  $P_N^0, P_N$  are projections increasing to  $I$  (i.e.  $P_N^0, P_N \uparrow I$ ).

- Applying the above results we show that

$$\begin{aligned} & \text{Tr}\left\{\left(\phi(H_1) - \phi(H_1^0)\right)\left(\psi(H_2) - \psi(H_2^0)\right)\right\} \\ &= \lim_{N \rightarrow \infty} \text{Tr}\left\{P_N\left(\phi(H_1^{(N)}) - \phi(H_1^{0(N)})\right)P_N^0\left(\psi(H_2^{(N)}) - \psi(H_2^{0(N)})\right)\right\}, \end{aligned} \quad (4)$$

for  $\phi, \psi \in \mathcal{P}([a, b])$ .

- **(Finite Dimensional Trace formula):** Using Theorem 2 we get

$$\begin{aligned}
 & \text{Tr} \left\{ P_N \left( \phi(H_1^{(N)}) - \phi(H_1^{0(N)}) \right) P_N^0 \left( \psi(H_2^{(N)}) - \psi(H_2^{0(N)}) \right) \right\} \\
 &= \int_a^b \int_a^b \phi'(x) \psi'(y) \xi_N(x, y) \, dx dy \\
 &= \int_{[a,b]^2} \phi'(x) \psi'(y) \mu_N(dx \times dy),
 \end{aligned} \tag{5}$$

where

$$\xi_N(x, y) = \text{Tr} \left\{ P_N \left[ E_{H_1^{(N)}}(x) - E_{H_1^{0(N)}}(x) \right] P_N^0 \left[ E_{H_2^{(N)}}(y) - E_{H_2^{0(N)}}(y) \right] P_N \right\}$$

and  $\mu_N$  is a complex Borel measure on  $[a, b]^2$  such that

$$\mu_N(\Delta) = \int_{\Delta} \xi_N(x, y) \, dx dy, \quad \text{for a Borel subset } \Delta \subseteq [a, b]^2.$$

- **(Finite Dimensional Trace formula):** Moreover, using Theorem 3 we have that

$$\begin{aligned} & \text{Tr} \left\{ P_N \left( \phi(H_1^{(N)}) - \phi(H_1^{0(N)}) \right) P_N^0 \left( \psi(H_2^{(N)}) - \psi(H_2^{0(N)}) \right) \right\} \\ &= \int_{[a,b]^2} \int_{[a,b]^2} \left\{ \frac{\phi(x_1) - \phi(x_2)}{x_1 - x_2} \right\} \left\{ \frac{\psi(y_1) - \psi(y_2)}{y_1 - y_2} \right\} \bullet \\ & \quad \left\langle P_N^0 V_1^{(N)} P_N, P_N^0 E_{\underline{H}^{0(N)}}(dx_2 \times dy_1) V_2^{(N)} E_{\underline{H}^{(N)}}(dx_1 \times dy_2) P_N \right\rangle_2, \end{aligned} \tag{6}$$

where  $V_j^{(N)} = H_j^{(N)} - H_j^{0(N)}$  for  $j = 1, 2$  and  $E_{\underline{H}^{0(N)}}(dx_2 \times dy_1) = E_{H_1^{0(N)}}(dx_2) E_{H_2^{0(N)}}(dy_1)$  and  $E_{\underline{H}^{(N)}}(dx_1 \times dy_2) = E_{H_1^{(N)}}(dx_1) E_{H_2^{(N)}}(dy_2)$  are  $\mathcal{B}_2(\mathcal{H})$ -valued spectral measures of the operators tuples  $\underline{H}^{0(N)}$  and  $\underline{H}^{(N)}$  respectively on the Borel sets of  $[a, b]^2$ .

- Combining (5) and (6) we get

$$\begin{aligned}
 & \int_{[a,b]^2} \Psi(x, y) \mu_N(dx \times dy) \\
 &= \int_{[a,b]^2} \int_{[a,b]^2} \left\{ \frac{\phi(x_1) - \phi(x_2)}{x_1 - x_2} \right\} \left\{ \frac{\psi(y_1) - \psi(y_2)}{y_1 - y_2} \right\} \bullet \\
 & \quad \left\langle P_N^0 V_1^{(N)} P_N, P_N^0 E_{\underline{H}^{0(N)}}(dx_2 \times dy_1) V_2^{(N)} E_{\underline{H}^{(N)}}(dx_1 \times dy_2) P_N \right\rangle_2 \\
 &= \int_{[a,b]^2} \int_{[a,b]^2} \frac{\int_{x_2}^{x_1} \int_{y_2}^{y_1} \Psi(x, y) dx dy}{(x_1 - x_2)(y_1 - y_2)} \bullet \\
 & \quad \left\langle P_N^0 V_1^{(N)} P_N, P_N^0 E_{\underline{H}^{0(N)}}(dx_2 \times dy_1) V_2^{(N)} E_{\underline{H}^{(N)}}(dx_1 \times dy_2) P_N \right\rangle_2,
 \end{aligned}$$

where  $\Psi(x, y) = \phi'(x)\psi'(y)$  and  $\phi, \psi \in \mathcal{P}([a, b])$ .

- For fixed  $N$ , we can extend the above equality to an arbitrary polynomial  $\Psi$  in two variables by taking suitable linear combination of products of polynomials in one-variables,  $x$  and  $y$  and then extend the above equality from  $\mathcal{P}([a, b]^2)$  to  $C([a, b]^2)$  by Stone-Weierstrass theorem.
- Next we show that for all  $\Psi \in C([a, b]^2)$ ,

$$\left| \int_{[a,b]^2} \Psi(x, y) \mu_N(dx \times dy) \right| < C \|\Psi\|_\infty,$$

for some constant  $C (< \infty)$  and hence by applying Helley's theorem we conclude that there exists a subsequence  $\mu_{N_k}$  of  $\mu_N$  such that  $\mu_{N_k}$  converges weakly to a unique complex Borel measure  $\mu$  on  $[a, b]^2$ , that is,

$$\lim_{k \rightarrow \infty} \int_{[a,b]^2} \Psi(x, y) \mu_{N_k}(dx \times dy) = \int_{[a,b]^2} \Psi(x, y) \mu(dx \times dy) \quad \forall \Psi \in C([a, b]^2).$$

## Regarding Absolute Continuity of the Measure $\mu$ :

- Unlike in one variable Krein's trace formula we note that the measure  $\mu$  which appears in Theorem 5 is not necessarily absolutely continuous with respect to the Lebesgue measure on  $\mathbb{R}^2$ . In fact the measure  $\mu$  may be singular with respect to the product Lebesgue measure on  $\mathbb{R}^2$  as shown in Theorem 6.
- Indeed, if we assume that the measure  $\mu$  is absolutely continuous with respect to the Lebesgue measure on  $\mathbb{R}^2$ , then there exists a function  $\xi \in L^1([a, b]^2)$  such that  $\mu(dx \times dy) = \xi(x, y)dxdy$ .
- Next from the main theorem (Theorem 4) in particular situation where  $H_1 = H_2 = H$  and  $H_1^0 = H_2^0 = H^0$  we get

$$\begin{aligned} & \text{Tr} \left\{ \left( \phi(H) - \phi(H^0) \right) \left( \psi(H) - \psi(H^0) \right) \right\} \\ &= \int_a^b \int_a^b \phi'(x) \psi'(y) \xi(x, y) dx dy, \end{aligned} \tag{7}$$

where  $\phi, \psi \in \mathcal{P}([a, b])$ .



- On the other hand we will show separately in the next theorem below (a counterexample theorem) that

$$\mathrm{Tr}\left\{\left(\phi(H)-\phi(H^0)\right)\left(\psi(H)-\psi(H^0)\right)\right\} = \int_a^b \phi'(t) \psi'(t) \eta(t) dt, \quad (8)$$

for suitable  $\phi, \psi \in \mathcal{P}([a, b])$ .

- Combining (7) and (8) we conclude that

$$\xi(x, y) = \delta(x - y) \eta(y),$$

which contradicts the fact that  $\xi \in L^1([a, b]^2)$  and hence the measure  $\mu$  is not absolutely continuous.

- Before going to discuss counterexample theorem in an infinite dimensional setup let us start with the similar type of theorem in finite dimension.

### Theorem 5

Let  $H$  and  $H^0$  be two self-adjoint operators in a finite dimensional Hilbert space  $\mathcal{H}$  such that  $\sigma(H) \cup \sigma(H^0) \subseteq [a, b]$ . Then the trace formula

$$\mathrm{Tr}\left\{\left(\psi(H) - \psi(H^0)\right)\left(\phi(H) - \phi(H^0)\right)\right\} = \int_a^b \psi'(t) \phi'(t) \eta(t) dt$$

holds for a suitable class of functions  $\phi, \psi : [a, b] \mapsto \mathbb{R}$  in  $C^1([a, b])$  and

$$\eta(t) = \mathrm{Tr}\left\{\left(H - H^0\right)\left(E_{H^0}(t) - E_H(t)\right)\right\}.$$

## Sketch of the Proof of Theorem 5:

- By spectral theorem and performing integration by-parts we get

$$\text{Tr}\left\{\left(H - H^0\right)\left(\phi(H) - \phi(H^0)\right)\right\} = \int_a^b \phi'(t) \eta(t) dt,$$

where  $\eta(t) = \text{Tr}\left\{\left(H - H^0\right)\left(E_{H^0}(t) - E_H(t)\right)\right\}$  and  $\phi$  is a real-valued continuously differentiable function on  $[a, b]$ .

- Next consider the real-valued continuously differentiable function  $\psi : [a, b] \rightarrow [\psi(a), \psi(b)]$  such that  $\psi' \neq 0$ . Moreover,  $\psi$  is invertible and  $\psi^{-1}$  is also continuously differentiable.
- Now let  $G^0 = \psi(H^0)$  and  $G = \psi(H)$ . Then both  $G$  and  $G^0$  are bounded self-adjoint operators and therefore by applying the above argument to  $G, G^0$  and interchanging the spectral variable  $\lambda = \psi(t)$  of  $G, G^0$  to the spectral variable  $t$  of  $H, H^0$  we conclude

$$\begin{aligned}
& \text{Tr} \left\{ \left( \psi(H) - \psi(H^0) \right) \left( \phi(H) - \phi(H^0) \right) \right\} \\
&= \text{Tr} \left\{ \left( G - G^0 \right) \left( \phi \circ \psi^{-1}(G) - \phi \circ \psi^{-1}(G^0) \right) \right\} \\
&= \int_a^b \phi'(t) \tilde{\eta}(\psi; t) dt,
\end{aligned} \tag{9}$$

where

$$\tilde{\eta}(\psi; t) = \text{Tr} \left\{ \left( \psi(H) - \psi(H^0) \right) \left( E_{H^0}(t) - E_H(t) \right) \right\},$$

and once again by performing integration by-parts and using the spectral theorem we conclude

$$\int_a^b \tilde{\eta}(\psi; t) dt = \int_a^b \psi'(t) \eta(t) dt.$$

- Finally by considering the function

$$\tilde{\psi}(t) = \begin{cases} \psi(t) & \text{for } a \leq t \leq \alpha \\ \psi(\alpha) & \text{for } \alpha \leq t \leq b, \end{cases}$$

where  $a \leq \alpha \leq b$  and noting the fact that  $\tilde{\eta}(\tilde{\psi}; t) = \tilde{\eta}(\psi; t)$  for  $a \leq t \leq \alpha$  and  $\tilde{\eta}(\tilde{\psi}; t) = 0$  for  $\alpha \leq t \leq b$  we conclude that

$$\int_a^\alpha \psi'(t) \eta(t) dt = \int_a^\alpha \tilde{\eta}(\psi; t) dt,$$

and thus  $\tilde{\eta}(\psi; t) = \psi'(t) \eta(t)$  almost everywhere and therefore the result follows by combining with equation (9).

# Counterexample Theorem:

## Theorem 6

Let  $H$  and  $H^0$  be two bounded self-adjoint operators in an infinite dimensional Hilbert space  $\mathcal{H}$  such that  $H - H^0 = V \in \mathcal{B}_2(\mathcal{H})$  and

$\sigma(H) \cup \sigma(H^0) \subseteq [a, b]$ . Then there exists a function  $\eta \in L^1([a, b])$  such that

$$\mathrm{Tr} \left\{ \left( \phi(H) - \phi(H^0) \right) \left( \psi(H) - \psi(H^0) \right) \right\} = \int_a^b \phi'(t) \psi'(t) \eta(t) dt, \quad (10)$$

for a suitable class of functions  $\phi, \psi : [a, b] \mapsto \mathbb{R}$  in  $C^1([a, b])$ .

## Sketch of the Proof of Theorem 6:

- **(Finite Dimensional Reduction):**

- ▶ Using Weyl-Von Neumann theorem we conclude that there exists a sequence  $\{P_N\}$  of finite rank projections such that

$$\|(I - P_N)H^0P_N\|_2, \|(I - P_N)V\|_2, \|(I - P_N)HP_N\|_2 \longrightarrow 0 \quad (11)$$

as  $N \longrightarrow \infty$ .

- ▶ Using the above results we show that

$$\begin{aligned} & \text{Tr}\left\{\left(\phi(H) - \phi(H^0)\right)\left(\psi(H) - \psi(H^0)\right)\right\} \\ &= \lim_{N \rightarrow \infty} \text{Tr}\left\{P_N\left(\phi(P_NHP_N) - \phi(P_NH^0P_N)\right)\right. \\ & \qquad \qquad \qquad \left.P_N\left(\psi(P_NHP_N) - \psi(P_NH^0P_N)\right)P_N\right\}, \end{aligned}$$

for  $\phi, \psi \in \mathcal{P}([a, b])$ .

- **(Finite Dimensional Formula):**

Using Theorem 5 we conclude that for a suitable class of functions

$$\phi, \psi : [a, b] \mapsto \mathbb{R},$$

$$\begin{aligned} & \text{Tr} \left\{ P_N \left( \phi(P_N H P_N) - \phi(P_N H^0 P_N) \right) \right. \\ & \qquad \qquad \qquad \left. P_N \left( \psi(P_N H P_N) - \psi(P_N H^0 P_N) \right) P_N \right\} \\ &= \int_a^b \phi'(t) \psi'(t) \eta_N(t) dt, \end{aligned}$$

where

$$\eta_N(t) = \text{Tr} \left\{ P_N \left( P_N H P_N - P_N H^0 P_N \right) P_N \left( E_{P_N H^0 P_N}(t) - E_{P_N H P_N}(t) \right) \right\}.$$



- Finally to guarantee the existence of the function  $\eta \in L^1([a, b])$  we show that the sequence  $\{\eta_N\}$  is a Cauchy sequence in  $L^1([a, b])$ . Indeed, we have shown that for  $f \in L^\infty([a, b])$  and

$$g(t) = \int_a^t f(\lambda) d\lambda,$$

$$\begin{aligned} & \|\eta_N - \eta_M\|_{L^1([a,b])} \\ &= \sup_{0 \neq f \in L^\infty([a,b])} \frac{\left| \int_a^b f(t) [\eta_N(t) - \eta_M(t)] dt \right|}{\|f\|_\infty} \\ &\leq \|V\|_2 \left\{ \|P_N H(I - P_N)\|_2 + \|P_N H^0(I - P_N)\|_2 + \|P_M H(I - P_M)\|_2 \right. \\ &\quad \left. + \|P_M H^0(I - P_M)\|_2 + \|P_N V P_N - P_M V P_M\|_2 \right\}, \end{aligned}$$

which converges to zero as  $N, M \rightarrow \infty$  (by (11)) and therefore  $\{\eta_N\}$  is a Cauchy sequence in  $L^1([a, b])$ .

## Remark

*In the counterexample theorem (Theorem 6) we can extend the theorem for any  $\phi, \psi \in C^1([a, b])$ . The only restriction of the function  $\psi$  in Theorem 6 is the following:  $\psi' \neq 0$  and  $\psi^{-1} \in C^1([a, b])$ . Now if we assume that  $\psi' = 0$  for some subset of  $[a, b]$ , then since  $\psi$  is continuously differentiable  $\psi' = 0$  on some interval  $\Delta \subseteq [a, b]$  and hence  $\psi$  is constant on  $\Delta$ . Let  $\Delta^c = \bigcup_{i=1}^{\infty} \delta_i$  where  $\delta_i$  is an interval of  $[a, b]$  for  $i \geq 1$  and*

*consider the function  $\tilde{\psi}|_{\Delta^c} = \sum_{i=1}^{\infty} \psi|_{\delta_i}$ . Therefore by applying Theorem 6*

*corresponding to the function  $\tilde{\psi}|_{\Delta^c}$  we will have the final conclusion because both left hand side and right hand side of (10) are equals to zero whenever  $\psi$  is constant.*

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**THANK YOU**