

Third order trace formula

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Abstract. In *J. Funct. Anal.* **257** (2009) 1092–1132, Dykema and Skripka showed the existence of higher order spectral shift functions when the unperturbed self-adjoint operator is bounded and the perturbation is Hilbert–Schmidt. In this article, we give a different proof for the existence of spectral shift function for the third order when the unperturbed operator is self-adjoint (bounded or unbounded, but bounded below).

Keywords. Trace formula; spectral shift function; perturbations of self-adjoint operators.

1. Introduction

Notations. Here, \mathcal{H} will denote the separable Hilbert space we work in; $\mathcal{B}(\mathcal{H})$, $\mathcal{B}_p(\mathcal{H})$ [$p \geq 1$], the set of bounded, Schatten p -class operators in \mathcal{H} respectively with $\|\cdot\|$, $\|\cdot\|_p$ as the associated norms. In particular, $\mathcal{B}_1(\mathcal{H})$ and $\mathcal{B}_2(\mathcal{H})$ are known as the set of trace class and Hilbert–Schmidt class operators in \mathcal{H} . Let A be a self-adjoint operator in \mathcal{H} with $\sigma(A)$ as the spectra and $E_A(\lambda)$ the spectral family. The symbols $\text{Dom}(A)$, $\text{Ker}(A)$, $\text{Ran}(A)$ and $\text{Tr}A$ denote the domain, kernel, range and trace of the operator A respectively.

Let A (possibly unbounded) and V be two self-adjoint operators in \mathcal{H} such that $V \in \mathcal{B}_1(\mathcal{H})$. Then Krein [10,11] proved that there exists a unique real-valued $L^1(\mathbb{R})$ -function ξ with support in the interval $[a, b]$ (where $a = \min\{\inf \sigma(A + V), \inf \sigma(A)\}$ and $b = \max\{\sup \sigma(A + V), \sup \sigma(A)\}$) such that

$$\text{Tr}[\phi(A + V) - \phi(A)] = \int_a^b \phi'(\lambda)\xi(\lambda)d\lambda, \quad (1.1)$$

for a large class of functions ϕ . The function ξ is known as Krein's spectral shift function and the relation (1.1) is called Krein's trace formula. In 1985, Voiculescu approached the trace formula (1.1) from a different direction. Later Voiculescu [18], and Sinha and Mohapatra [13,14] proved that

$$\begin{aligned} \text{Tr}[\phi(A + V) - \phi(A)] &= \lim_{n \rightarrow \infty} \text{Tr}_n [\phi((A + V)_n) - \phi(A_n)] \\ &= \int \phi'(\lambda)\xi(\lambda)d\lambda, \end{aligned} \quad (1.2)$$

by adapting the Weyl–von Neumann’s theorem (where $\phi(\cdot)$ is a suitable function and $(A + V)_n, A_n$ are finite dimensional approximations of $(A + V)$ and A respectively and Tr_n is the associated finite dimensional trace). In [9], Koplienko considers instead $\phi(A + V) - \phi(A) - D^{(1)}\phi(A)(V)$, where $D^{(1)}\phi(A)$ denotes the first-order Fréchet derivative of ϕ at A [2] and found a trace formula for this expression. If $V \in \mathcal{B}_2(\mathcal{H})$, then Koplienko’s formula asserts that there exists a unique function $\eta \in L^1(\mathbb{R})$ such that

$$\text{Tr}\{\phi(A + V) - \phi(A) - D^{(1)}\phi(A)(V)\} = \int_{-\infty}^{\infty} \phi''(\lambda)\eta(\lambda)d\lambda \tag{1.3}$$

for rational functions ϕ with poles off \mathbb{R} . In [5,16], Koplienko’s trace formula was derived using finite dimensional approximation method, while Dykema and Skripka [6] obtained the formula (1.3) in the semi-finite von Neumann algebra setting and also studied the existence of higher order spectral shift functions. In Theorem 5.1 of [6], Dykema and Skripka showed that for a self-adjoint operator A (possibly unbounded) and a self-adjoint operator $V \in \mathcal{B}_2(\mathcal{H})$, the following assertions hold:

(i) *There is a unique finite real-valued measure ν_3 on \mathbb{R} such that the trace formula*

$$\begin{aligned} \text{Tr}\{\phi(A + V) - \phi(A) - D^{(1)}\phi(A)(V) - \frac{1}{2}D^{(2)}\phi(A)(V, V)\} \\ = \int_{-\infty}^{\infty} \phi'''(\lambda)d\nu_3(\lambda), \end{aligned} \tag{1.4}$$

holds for suitable functions ϕ , where $D^{(2)}\phi(A)$ is the second order Fréchet derivative of ϕ at A [2]. The total variation of ν_3 is bounded by $\frac{1}{3!}\|V\|_2^3$.

(ii) *If, in addition, A is bounded, then ν_3 is absolutely continuous.*

It is to be noted that the main results of this article (Theorems 2.6 and 3.3) have been obtained in [12], under the condition that $V \in \mathcal{B}_3(\mathcal{H})$ and with more general setting. However, the method employed here seems to be simpler and moreover, we get more explicit expressions for the shift function.

This paper is organized as follows. In § 2, we establish the formula (1.4) for bounded self-adjoint case and § 3 is devoted to the unbounded self-adjoint case.

2. Bounded case

The next three lemmas are preparatory for the proof of the main theorem of this section, Theorem 2.6.

Lemma 2.1. Let, for a given $n \in \mathbb{N}$, $\{a_k\}_{k=0}^{n-1}$ be a sequence of complex numbers such that $a_{n-k-1} = a_k$. Then

$$\sum_{j=0}^{n-1} \sum_{k=0}^{n-j-1} a_k + \sum_{j=1}^n \sum_{k=0}^{j-1} a_k = (n + 1) \sum_{k=0}^{n-1} a_k.$$

Proof. By changing the indices of summation and using the fact that $a_{n-k-1} = a_k$, we get

$$\begin{aligned}
\sum_{j=0}^{n-1} \sum_{k=0}^{n-j-1} a_k + \sum_{j=1}^n \sum_{k=0}^{j-1} a_k &= \sum_{j=0}^{n-1} \sum_{k=j}^{n-1} a_{n-k-1} + \sum_{j=0}^{n-1} \sum_{k=0}^j a_k \\
&= \sum_{j=0}^{n-1} \sum_{k=j}^{n-1} a_k + \sum_{j=0}^{n-1} \sum_{k=0}^j a_k \\
&= \sum_{j=0}^{n-1} a_j + \sum_{j=0}^{n-1} \sum_{k=0}^{n-1} a_k \\
&= \sum_{j=0}^{n-1} a_j + n \sum_{k=0}^{n-1} a_k \\
&= (n+1) \sum_{k=0}^{n-1} a_k.
\end{aligned}$$

□

Lemma 2.2. Let A and V be two bounded self-adjoint operators in an infinite dimensional Hilbert space \mathcal{H} such that $V \in \mathcal{B}_3(\mathcal{H})$. Let $p(\lambda) = \lambda^r$ ($r \geq 0$). Then

$$\begin{aligned}
&\text{Tr} \left[(A+V)^r - A^r - D^{(1)}(A^r)(V) - \frac{1}{2} D^{(2)}(A^r)(V, V) \right] \\
&= r \sum_{k=0}^{r-2} \int_0^1 ds \int_0^s d\tau \text{Tr} [V A_\tau^{r-k-2} V A_\tau^k - V A^{r-k-2} V A^k], \tag{2.1}
\end{aligned}$$

where $A_\tau = A + \tau V$ and $0 \leq \tau \leq 1$.

Proof. For $X \in \mathcal{B}(\mathcal{H})$, $p(A+X) - p(A) = \sum_{j=0}^{r-1} (A+X)^{r-j-1} X A^j$ and hence

$$\begin{aligned}
&\left\| p(A+X) - p(A) - \sum_{j=0}^{r-1} A^{r-j-1} X A^j \right\| \\
&\leq \sum_{j=0}^{r-2} \sum_{k=0}^{r-j-2} \|A+X\|^{r-j-k-2} \|X\| \|A\|^k \|X\| \|A\|^j,
\end{aligned}$$

proving that $D^{(1)}(A^r)(X) = \sum_{j=0}^{r-1} A^{r-j-1} X A^j$.

Again for $X, Y \in \mathcal{B}(\mathcal{H})$,

$$\begin{aligned}
& D^{(1)}((A+X)^r)(Y) - D^{(1)}(A^r)(Y) \\
&= \sum_{j=0}^{r-1} (A+X)^{r-j-1} Y (A+X)^j - \sum_{j=0}^{r-1} A^{r-j-1} Y A^j \\
&= \sum_{j=0}^{r-1} [(A+X)^{r-j-1} - A^{r-j-1}] Y (A+X)^j \\
&\quad + \sum_{j=0}^{r-1} A^{r-j-1} Y [(A+X)^j - A^j] \\
&= \sum_{j=0}^{r-2} \sum_{k=0}^{r-j-2} (A+X)^{r-j-k-2} X A^k Y (A+X)^j \\
&\quad + \sum_{j=1}^{r-1} \sum_{k=0}^{j-1} A^{r-j-1} Y (A+X)^k X A^{j-k-1},
\end{aligned}$$

leading to the estimate

$$\begin{aligned}
& \left\| D^{(1)}((A+X)^r)(Y) - D^{(1)}(A^r)(Y) \right. \\
& \quad \left. - \left(\sum_{j=0}^{r-2} \sum_{k=0}^{r-j-2} A^{r-j-k-2} X A^k Y A^j + \sum_{j=1}^{r-1} \sum_{k=0}^{j-1} A^{r-j-1} Y A^k X A^{j-k-1} \right) \right\| \\
&= \mathcal{O}(\|X\|^2),
\end{aligned}$$

for $\|X\| \leq 1$, proving that

$$\begin{aligned}
D^{(2)}(A^r)(X, Y) &= \sum_{j=0}^{r-2} \sum_{k=0}^{r-j-2} A^{r-j-k-2} X A^k Y A^j \\
&\quad + \sum_{j=1}^{r-1} \sum_{k=0}^{j-1} A^{r-j-1} Y A^k X A^{j-k-1}. \tag{2.2}
\end{aligned}$$

Recall that $A_s = A + sV \in \mathcal{B}_{s,a}(\mathcal{H})$ ($0 \leq s \leq 1$), and a similar calculation shows that the map $[0, 1] \ni s \mapsto A_s^r$ is continuously differentiable in norm-topology and

$$\frac{d}{ds}(A_s^r) = \sum_{j=0}^{r-1} A_s^{r-j-1} V A_s^j = \sum_{j=0}^{r-1} A_s^j V A_s^{r-j-1}.$$

Hence

$$\begin{aligned}
(A + V)^r - A^r - D^{(1)}(A^r)(V) &= \int_0^1 ds \frac{d}{ds} (A_s^r) - D^{(1)}(A^r)(V) \\
&= \int_0^1 ds \sum_{j=0}^{r-1} (A_s^{r-j-1} V A_s^j - A^{r-j-1} V A^j) \\
&= \int_0^1 ds \sum_{j=0}^{r-1} \int_0^s d\tau \frac{d}{d\tau} (A_\tau^{r-j-1} V A_\tau^j),
\end{aligned}$$

which by an application of Leibnitz's rule reduces to

$$\int_0^1 ds \int_0^s d\tau \left(\sum_{j=0}^{r-2} \sum_{k=0}^{r-j-2} A_\tau^{r-j-k-2} V A_\tau^k V A_\tau^j + \sum_{j=1}^{r-1} \sum_{k=0}^{j-1} A_\tau^{r-j-1} V A_\tau^k V A_\tau^{j-k-1} \right)$$

and using (2.2), we get

$$\begin{aligned}
(A + V)^r - A^r - D^{(1)}(A^r)(V) - \frac{1}{2} D^{(2)}(A^r)(V, V) \\
= \int_0^1 ds \int_0^s d\tau \left\{ \sum_{j=0}^{r-2} \sum_{k=0}^{r-j-2} A_\tau^{r-j-k-2} V A_\tau^k V A_\tau^j \right. \\
+ \sum_{j=1}^{r-1} \sum_{k=0}^{j-1} A_\tau^{r-j-1} V A_\tau^k V A_\tau^{j-k-1} - \sum_{j=0}^{r-2} \sum_{k=0}^{r-j-2} A_\tau^{r-j-k-2} V A^k V A^j \\
\left. - \sum_{j=1}^{r-1} \sum_{k=0}^{j-1} A_\tau^{r-j-1} V A^k V A^{j-k-1} \right\}. \tag{2.3}
\end{aligned}$$

Let us denote the sum of the first and third term inside the integral in (2.3) to be

$$\begin{aligned}
I_1 &\equiv \sum_{j=0}^{r-2} \sum_{k=0}^{r-j-2} [A_\tau^{r-j-k-2} V A_\tau^k V A_\tau^j - A_\tau^{r-j-k-2} V A^k V A^j] \\
&= \sum_{j=0}^{r-2} \sum_{k=0}^{r-j-2} [A_\tau^{r-j-k-2} - A_\tau^{r-j-k-2}] V A_\tau^k V A_\tau^j \\
&\quad + \sum_{j=0}^{r-2} \sum_{k=0}^{r-j-2} A_\tau^{r-j-k-2} V [A_\tau^k - A^k] V A_\tau^j \\
&\quad + \sum_{j=0}^{r-2} \sum_{k=0}^{r-j-2} A_\tau^{r-j-k-2} V A^k V [A_\tau^j - A^j] \in \mathcal{B}_1(\mathcal{H}),
\end{aligned}$$

since $V \in \mathcal{B}_3(\mathcal{H})$ and $A_\tau^k - A^k \in \mathcal{B}_3(\mathcal{H}) \forall \tau \in [0, 1]$ and $k \in \{0, 1, 2, 3, \dots\}$. Thus by the cyclicity of trace, we have that

$$\text{Tr}(\mathbf{I}_1) = \sum_{j=0}^{r-2} \sum_{k=0}^{r-j-2} \text{Tr}[A_\tau^{r-k-2} V A_\tau^k V - A^{r-k-2} V A^k V].$$

Again if we set the sum of the second and fourth term inside the integral in (2.3) to be

$$\mathbf{I}_2 \equiv \sum_{j=1}^{r-1} \sum_{k=0}^{j-1} [A_\tau^{r-j-1} V A_\tau^k V A_\tau^{j-k-1} - A^{r-j-1} V A^k V A^{j-k-1}] \in \mathcal{B}_1(\mathcal{H}),$$

a similar calculation shows that

$$\text{Tr}(\mathbf{I}_2) = \sum_{j=1}^{r-1} \sum_{k=0}^{j-1} \text{Tr}[A_\tau^{r-k-2} V A_\tau^k V - A^{r-k-2} V A^k V].$$

By applying Lemma 2.1 with $n = r - 1$ and $a_k = \text{Tr}[A_\tau^{r-k-2} V A_\tau^k V - A^{r-k-2} V A^k V]$ and using the cyclicity of trace, we conclude that

$$\begin{aligned} \text{Tr}(\mathbf{I}_1) + \text{Tr}(\mathbf{I}_2) &= r \sum_{k=0}^{r-2} \text{Tr}[A_\tau^{r-k-2} V A_\tau^k V - A^{r-k-2} V A^k V] \\ &= r \sum_{k=0}^{r-2} \text{Tr}[V A_\tau^{r-k-2} V A_\tau^k - V A^{r-k-2} V A^k]. \end{aligned} \quad (2.4)$$

Hence combining (2.3) and (2.4), we get the required expression (2.1). \square

Remark 2.3. Though the expressions for Fréchet derivatives of a class of functions were derived in [1] in terms of divided differences, here the expression for the trace of the remainder term in (2.1) is different and simpler.

Lemma 2.4. Let B be a bounded operator in an infinite dimensional Hilbert space \mathcal{H} (i.e. $B \in \mathcal{B}(\mathcal{H})$). Define $\mathcal{M}_B : \mathcal{B}_2(\mathcal{H}) \mapsto \mathcal{B}_2(\mathcal{H})$ (looking upon $\mathcal{B}_2(\mathcal{H}) \equiv \tilde{\mathcal{H}}$ as a Hilbert space with inner product given by trace i.e. $\langle X, Y \rangle_2 = \text{Tr}\{X^* Y\}$ for $X, Y \in \mathcal{B}_2(\mathcal{H})$) by $\mathcal{M}_B(X) = BX - XB$; $X \in \mathcal{B}_2(\mathcal{H})$. Then

- (i) \mathcal{M}_B is a bounded operator on $\tilde{\mathcal{H}}$ (i.e. $\mathcal{M}_B \in \mathcal{B}(\tilde{\mathcal{H}})$) with $\mathcal{M}_B^* = \mathcal{M}_{B^*}$.
- (ii) $\text{Ker}(\mathcal{M}_B)$ and its orthogonal complement $\overline{\text{Ran}(\mathcal{M}_{B^*})}$ in $\tilde{\mathcal{H}}$ are left invariant by left and right multiplication by B^n and $(B^*)^n$ ($n = 1, 2, 3, \dots$) respectively.
- (iii) $\tilde{\mathcal{H}} = \text{Ker}(\mathcal{M}_B) \oplus \overline{\text{Ran}(\mathcal{M}_{B^*})}$; $\mathcal{B}_2(\mathcal{H}) \ni X = X_1 \oplus X_2$, where $X_1 \in \text{Ker}(\mathcal{M}_B)$ and $X_2 \in \overline{\text{Ran}(\mathcal{M}_{B^*})}$.
- (iv) If $\text{Ker}(\mathcal{M}_B) = \text{Ker}(\mathcal{M}_{B^*})$, then $\text{Ker}(\mathcal{M}_B)$ and $\overline{\text{Ran}(\mathcal{M}_B)}$ are generated by their self-adjoint elements and for $X \in \tilde{\mathcal{H}}$, we have $(X^*)_1 = X_1^*$ and $(X^*)_2 = X_2^*$, where $X = X_1 \oplus X_2$ and $X^* = (X^*)_1 \oplus (X^*)_2$ are the respective decompositions of X and X^* in $\tilde{\mathcal{H}}$.

- (v) If $\text{Ker}(\mathcal{M}_B) = \text{Ker}(\mathcal{M}_{B^*})$, then for $X = X^* \in \tilde{\mathcal{H}}$, $X = X_1 \oplus X_2$ with X_1 and X_2 both self-adjoint.
- (vi) (a) For $B = B^* \in \mathcal{B}(\mathcal{H})$, \mathcal{M}_B is self-adjoint in $\tilde{\mathcal{H}}$ and for $X = X^* \in \tilde{\mathcal{H}}$, we have $X_1 = X_1^*$ and $X_2 = X_2^*$.
 (b) For $B = (A + i)^{-1}$ (where A is an unbounded self-adjoint operator in \mathcal{H}), \mathcal{M}_B is bounded normal in $\tilde{\mathcal{H}}$ and for $X = X^* \in \tilde{\mathcal{H}}$, we have $X_1 = X_1^*$ and $X_2 = X_2^*$, where $X = X_1 \oplus X_2$ is the decomposition of X in $\tilde{\mathcal{H}}$.
- (vii) (a) Let $[0, 1] \ni \tau \rightarrow A_\tau \in \mathcal{B}_{s,a}(\mathcal{H})$ (set of bounded self-adjoint operators in \mathcal{H}) be holomorphic in operator norm, and let $\tilde{\mathcal{H}} \ni X \equiv X_{1\tau} \oplus X_{2\tau}$ be the self-adjoint decomposition with respect to A_τ . Then $\tau \rightarrow X_{1\tau}, X_{2\tau} \in \tilde{\mathcal{H}}$ are continuous.
 (b) Let $\{A_\tau\}_{\tau \in [0,1]}$ be a family of unbounded self-adjoint operators in \mathcal{H} such that $[0, 1] \ni \tau \rightarrow (A_\tau + i)^{-1}$ is holomorphic in operator norm. Then the conclusions of (vii)(a) are valid for the decomposition of $\tilde{\mathcal{H}}$ with respect to $B_\tau \equiv (A_\tau + i)^{-1}$.

Proof. The proofs of (i) to (iii) are standard and for (iv), we note that since $\text{Ker}(\mathcal{M}_B) = \text{Ker}(\mathcal{M}_{B^*})$, $X \in \text{Ker}(\mathcal{M}_B)$ if and only if $X^* \in \text{Ker}(\mathcal{M}_B)$ and hence for any $X \in \text{Ker}(\mathcal{M}_B)$ can be written as $X = \left(\frac{X+X^*}{2}\right) + i\left(\frac{X-X^*}{2i}\right)$, proving that $\text{Ker}(\mathcal{M}_B)$ is generated by its self-adjoint elements. Similarly, by a similar argument we conclude that $\overline{\text{Ran}(\mathcal{M}_B)}$ is also generated by its self-adjoint elements.

Let $X \in \tilde{\mathcal{H}}$, and $X = X_1 \oplus X_2$ and $X^* = (X^*)_1 \oplus (X^*)_2$ be the corresponding decompositions of X and X^* in $\tilde{\mathcal{H}}$. Then for any $Y_1 = Y_1^* \in \text{Ker}(\mathcal{M}_B)$,

$$\langle X, Y_1 \rangle_2 = \langle X_1, Y_1 \rangle_2 = \text{Tr}\{X_1^* Y_1\} = \text{Tr}\{Y_1 X_1^*\} = \langle Y_1, X_1^* \rangle_2 = \overline{\langle X_1^*, Y_1 \rangle_2}.$$

But on the other hand,

$$\langle X, Y_1 \rangle_2 = \text{Tr}\{X^* Y_1\} = \text{Tr}\{(Y_1 X)^*\} = \overline{\text{Tr}\{Y_1 X\}} = \overline{\langle X^*, Y_1 \rangle_2} = \overline{\langle (X^*)_1, Y_1 \rangle_2}$$

and hence $\langle (X^*)_1 - X_1^*, Y_1 \rangle_2 = 0 \forall Y_1 = Y_1^* \in \text{Ker}(\mathcal{M}_B)$, which implies that $\langle (X^*)_1 - X_1^*, Y \rangle_2 = 0 \forall Y \in \text{Ker}(\mathcal{M}_B)$, proving that $(X^*)_1 = X_1^*$. Similarly, by the same argument we conclude that $(X^*)_2 = X_2^*$.

The results (v) and (vi(a)) follow from (iv) and (v) respectively. For (vi(b)), it suffices to note that any $X \in \mathcal{B}_2(\mathcal{H})$ commuting with $(A + i)^{-1}$ commutes with the spectral family $E_A(\cdot)$ of A .

For (vii(a)), since the map $[0, 1] \ni \tau \rightarrow \mathcal{M}_{A_\tau}$ is holomorphic, (using Theorem 1.8, page 370 of [8]) we conclude that the map $[0, 1] \ni \tau \rightarrow P_0(\tau)$ (where $P_0(\tau)$ is the projection onto $\text{Ker}(\mathcal{M}_{A_\tau})$) is continuous and since $X_{1\tau} \equiv P_0(\tau)X$ we get that the map $[0, 1] \ni \tau \rightarrow X_{1\tau}$ is continuous. Similarly, since the map $[0, 1] \ni \tau \rightarrow I - P_0(\tau)$ is continuous and $X_{2\tau} = (I - P_0(\tau))X$ we conclude that the map $[0, 1] \ni \tau \rightarrow X_{2\tau}$ is also continuous.

Conclusions of (vii(b)) follow immediately from (vii(a)) since the map $[0, 1] \ni \tau \rightarrow \mathcal{M}_{(A_\tau+i)^{-1}}$ is holomorphic, and since $\mathcal{M}_{(A_\tau+i)^{-1}}$ is normal for each τ . □

Remark 2.5. Let A and V be two bounded self-adjoint operators in an infinite dimensional Hilbert space \mathcal{H} such that $V \in \mathcal{B}_2(\mathcal{H})$ and let $A_\tau = A + \tau V$ ($0 \leq \tau \leq 1$). Then by Lemma 2.4 with $B = A$ and A_τ respectively to get $V = V_1 \oplus V_2 = V_{1\tau} \oplus V_{2\tau}$, with V_j and $V_{j\tau}$ ($j = 1, 2$) self-adjoint and therefore $\|V\|_2^2 = \|V_1\|_2^2 + \|V_2\|_2^2 = \|V_{1\tau}\|_2^2 + \|V_{2\tau}\|_2^2 \forall 0 \leq \tau \leq 1$.

Theorem 2.6. Let A and V be two bounded self-adjoint operators in an infinite dimensional Hilbert space \mathcal{H} such that $V \in \mathcal{B}_2(\mathcal{H})$. Then there exists a unique real-valued function $\eta \in L^1([a, b])$ such that

$$\begin{aligned} & \operatorname{Tr} \left[p(A+V) - p(A) - D^{(1)}p(A)(V) - \frac{1}{2}D^{(2)}p(A)(V, V) \right] \\ &= \int_a^b p'''(\lambda)\eta(\lambda)d\lambda, \end{aligned} \quad (2.5)$$

where $p(\cdot)$ is a polynomial in $[a, b]$, $a = [\inf \sigma(A) - \|V\|]$, $b = [\sup \sigma(A) + \|V\|]$ and $\int_a^b \eta(\lambda)d\lambda = \frac{1}{6}\operatorname{Tr}(V^3)$.

Remark 2.7. It is noted that while in [12, 15, 17], the method of multiple operator integrals is used to establish the formula (2.5), here we derive η as an L^1 -limit of a sequence $\{\eta_n\}$ which has an explicit expression in terms of A and V , with $V \in \mathcal{B}_2(\mathcal{H})$. For this Lemma 2.4 plays a crucial role.

Proof of Theorem 2.6. It will be sufficient to prove the theorem for $p(\lambda) = \lambda^r$ ($r \geq 0$). Note that for $r = 0, 1$ or 2 , both sides of (2.5) are identically zero. We set $A_\tau = A + \tau V$ and $0 \leq \tau \leq 1$. Then by Lemma 2.2, we have that

$$\begin{aligned} & \operatorname{Tr} \left[(A+V)^r - A^r - D^{(1)}(A^r)(V) - \frac{1}{2}D^{(2)}(A^r)(V, V) \right] \\ &= r \sum_{k=0}^{r-2} \int_0^1 ds \int_0^s d\tau \operatorname{Tr}[V A_\tau^{r-k-2} V A_\tau^k - V A^{r-k-2} V A^k] \\ &= r(r-1) \int_0^1 ds \int_0^s d\tau \operatorname{Tr}[V_{1\tau}^2 A_\tau^{r-2} - V_1^2 A^{r-2}] \\ &\quad + r \sum_{k=0}^{r-2} \int_0^1 ds \int_0^s d\tau \operatorname{Tr}[V_{2\tau} A_\tau^{r-k-2} V_{2\tau} A_\tau^k - V_2 A^{r-k-2} V_2 A^k], \end{aligned} \quad (2.6)$$

where we have also noted the invariance, orthogonality and continuity properties in Lemma 2.4(ii)–(vii) and set $V = V_1 \oplus V_2 = V_{1\tau} \oplus V_{2\tau} \in \mathcal{B}_2(\mathcal{H})$ as in Remark 2.5. Using the spectral families $E_\tau(\cdot)$ and $E(\cdot)$ of the self-adjoint operators A_τ and A respectively and integrating by parts, the first term of the expression (2.6) is equal to

$$\begin{aligned} & r(r-1) \int_0^1 ds \int_0^s d\tau \int_a^b \lambda^{r-2} \operatorname{Tr}[V_{1\tau}^2 E_\tau(d\lambda) - V_1^2 E(d\lambda)] \\ &= r(r-1) \int_0^1 ds \int_0^s d\tau \left\{ \lambda^{r-2} \operatorname{Tr}[V_{1\tau}^2 E_\tau(\lambda) - V_1^2 E(\lambda)] \Big|_{\lambda=a}^b \right. \\ &\quad \left. - \int_a^b (r-2)\lambda^{r-3} \operatorname{Tr}[V_{1\tau}^2 E_\tau(\lambda) - V_1^2 E(\lambda)]d\lambda \right\} \\ &= r(r-1)b^{r-2} \int_0^1 ds \int_0^s d\tau \operatorname{Tr}[V_{1\tau}^2 - V_1^2] \\ &\quad + r(r-1)(r-2) \int_0^1 ds \int_0^s d\tau \int_a^b \lambda^{r-3} \operatorname{Tr}[V_1^2 E(\lambda) - V_{1\tau}^2 E_\tau(\lambda)]d\lambda. \end{aligned} \quad (2.7)$$

Since $V_2 \in \overline{\text{Ran}(\mathcal{M}_A)}$, there exists a sequence $\{V_2^{(n)}\} \subseteq \text{Ran}(\mathcal{M}_A)$ such that $\|V_2^{(n)} - V_2\|_2 \rightarrow 0$ as $n \rightarrow \infty$ and $V_2^{(n)} = AY_0^{(n)} - Y_0^{(n)}A$, for a sequence $\{Y_0^{(n)}\} \subseteq \mathcal{B}_2(\mathcal{H})$. Similarly, for every $\tau \in (0, 1]$, there exists a sequence $\{V_{2\tau}^{(n)}\} \subseteq \text{Ran}(\mathcal{M}_{A_\tau})$ such that $\|V_{2\tau}^{(n)} - V_{2\tau}\|_2 \rightarrow 0$ point-wise as $n \rightarrow \infty$ and $V_{2\tau}^{(n)} = A_\tau Y^{(n)} - Y^{(n)}A_\tau$, for some sequence $\{Y^{(n)}\} \subseteq \mathcal{B}_2(\mathcal{H})$. Observe that $Y_0^{(n)}$ and $Y^{(n)}$ must be skew-adjoint for each n , since $V_2^{(n)}$ and $V_{2\tau}^{(n)}$ can be chosen to be self-adjoint. Furthermore, by Lemma 2.4(vii)(a), the map $[0, 1] \ni \tau \rightarrow V_{1\tau}, V_{2\tau}$ are continuous.

Hence the second term of the expression (2.6) is equal to

$$\begin{aligned} & r \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \sum_{k=0}^{r-2} \text{Tr}\{V_{2\tau} A_\tau^{r-k-2} V_{2\tau}^{(n)} A_\tau^k - V_2 A^{r-k-2} V_2^{(n)} A^k\} \\ &= r \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \sum_{k=0}^{r-2} \int_a^b \int_a^b \lambda^{r-k-2} \mu^k \\ &\quad \times \text{Tr}\{V_{2\tau} E_\tau(d\lambda) V_{2\tau}^{(n)} E_\tau(d\mu) - V_2 E(d\lambda) V_2^{(n)} E(d\mu)\} \\ &= r \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^b \int_a^b \phi(\lambda, \mu) \\ &\quad \times \text{Tr}\{V_{2\tau} E_\tau(d\lambda) V_{2\tau}^{(n)} E_\tau(d\mu) - V_2 E(d\lambda) V_2^{(n)} E(d\mu)\}, \end{aligned}$$

where $\phi(\lambda, \mu) = \frac{\lambda^{r-1} - \mu^{r-1}}{\lambda - \mu}$ if $\lambda \neq \mu$; $= (r-1)\lambda^{r-2}$ if $\lambda = \mu$, and where the interchange of the limit and the integration is justified by an application of the bounded convergence theorem. Furthermore using the representation of $V_{2\tau}^{(n)} \in \text{Ran}(\mathcal{M}_{A_\tau})$, the above reduces to

$$\begin{aligned} & r \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^b \int_a^b \phi(\lambda, \mu) \\ &\quad \times \text{Tr}\{V_{2\tau} E_\tau(d\lambda) [A_\tau Y^{(n)} - Y^{(n)} A_\tau] E_\tau(d\mu) \\ &\quad - V_2 E(d\lambda) [AY_0^{(n)} - Y_0^{(n)} A] E(d\mu)\} \\ &= r \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^b \int_a^b (\lambda^{r-1} - \mu^{r-1}) \\ &\quad \times \text{Tr}\{V_{2\tau} E_\tau(d\lambda) Y^{(n)} E_\tau(d\mu) - V_2 E(d\lambda) Y_0^{(n)} E(d\mu)\} \\ &= r \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^b \lambda^{r-1} \\ &\quad \times \text{Tr}\{V_{2\tau} [E_\tau(d\lambda), Y^{(n)}] - V_2 [E(d\lambda), Y_0^{(n)}]\}. \end{aligned} \tag{2.8}$$

Again by twice integrating by parts, the expression in (2.8) is equal to

$$\begin{aligned}
& r \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \left\{ \lambda^{r-1} \operatorname{Tr}(V_{2\tau}[E_\tau(\lambda), Y^{(n)}] - V_2[E(\lambda), Y_0^{(n)}]) \Big|_{\lambda=a}^b \right. \\
& \quad \left. - \int_a^b (r-1) \lambda^{r-2} \operatorname{Tr}(V_{2\tau}[E_\tau(\lambda), Y^{(n)}] - V_2[E(\lambda), Y_0^{(n)}]) d\lambda \right\} \\
& = -r(r-1) \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^b \lambda^{r-2} \\
& \quad \times \operatorname{Tr}\{V_{2\tau}[E_\tau(\lambda), Y^{(n)}] - V_2[E(\lambda), Y_0^{(n)}]\} d\lambda \\
& = -r(r-1) \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \left\{ \lambda^{r-2} \left(\int_a^\lambda \operatorname{Tr}(V_{2\tau}[E_\tau(\mu), Y^{(n)}] \right. \right. \\
& \quad \left. \left. - V_2[E(\mu), Y_0^{(n)}]) d\mu \right) \Big|_{\lambda=a}^b \right. \\
& \quad \left. + r(r-1) \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^b (r-2) \lambda^{r-3} \right. \\
& \quad \left. \times \left(\int_a^\lambda \operatorname{Tr}(V_{2\tau}[E_\tau(\mu), Y^{(n)}] - V_2[E(\mu), Y_0^{(n)}]) d\mu \right) d\lambda \right. \\
& = -r(r-1) b^{r-2} \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^b \operatorname{Tr}(V_{2\tau}[E_\tau(\mu), Y^{(n)}] \\
& \quad - V_2[E(\mu), Y_0^{(n)}]) d\mu + r(r-1)(r-2) \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^b \lambda^{r-3} \\
& \quad \times \left(\int_a^\lambda \operatorname{Tr}(V_{2\tau}[E_\tau(\mu), Y^{(n)}] - V_2[E(\mu), Y_0^{(n)}]) d\mu \right) d\lambda. \tag{2.9}
\end{aligned}$$

Next we note that by integration by parts,

$$\begin{aligned}
\operatorname{Tr}(V_{2\tau}^2 - V_2^2) & = \lim_{n \rightarrow \infty} \operatorname{Tr}(V_{2\tau} V_{2\tau}^{(n)} - V_2 V_2^{(n)}) \\
& = \lim_{n \rightarrow \infty} \operatorname{Tr}(V_{2\tau}[A_\tau, Y^{(n)}] - V_2[A, Y_0^{(n)}]) \\
& = \lim_{n \rightarrow \infty} \int_a^b \mu \operatorname{Tr}(V_{2\tau}[E_\tau(d\mu), Y^{(n)}] - V_2[E(d\mu), Y_0^{(n)}]) \\
& = \lim_{n \rightarrow \infty} \left[\mu \operatorname{Tr}(V_{2\tau}[E_\tau(\mu), Y^{(n)}] - V_2[E(\mu), Y_0^{(n)}]) \Big|_{\mu=a}^b \right. \\
& \quad \left. - \int_a^b \operatorname{Tr}(V_{2\tau}[E_\tau(\mu), Y^{(n)}] - V_2[E(\mu), Y_0^{(n)}]) d\mu \right].
\end{aligned}$$

The boundary term above vanishes and substituting the above in the first expression in (2.9), we get that the right-hand side of (2.9) is

$$r(r-1)b^{r-2} \int_0^1 ds \int_0^s d\tau \operatorname{Tr}(V_{2\tau}^2 - V_2^2) + r(r-1)(r-2) \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^b \lambda^{r-3} \eta_{2\tau}^{(n)}(\lambda) d\lambda,$$

where $\eta_{2\tau}^{(n)}(\lambda) = \int_a^\lambda \operatorname{Tr}(V_{2\tau}[E_\tau(\mu), Y^{(n)}] - V_2[E(\mu), Y_0^{(n)}]) d\mu$.

Hence

$$\begin{aligned} & r \sum_{k=0}^{r-2} \int_0^1 ds \int_0^s d\tau \operatorname{Tr}[V_{2\tau} A_\tau^{r-k-2} V_{2\tau} A_\tau^k - V_2 A^{r-k-2} V_2 A^k] \\ &= r(r-1)b^{r-2} \int_0^1 ds \int_0^s d\tau \operatorname{Tr}(V_{2\tau}^2 - V_2^2) \\ &+ r(r-1)(r-2) \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^b \lambda^{r-3} \eta_{2\tau}^{(n)}(\lambda) d\lambda. \end{aligned} \tag{2.10}$$

Combining (2.7) and (2.10) and since $\|V\|_2^2 = \operatorname{Tr}(V_{1\tau}^2 + V_{2\tau}^2) = \operatorname{Tr}(V_1^2 + V_2^2)$, we conclude that

$$\begin{aligned} & \operatorname{Tr} \left[(A + V)^r - A^r - D^{(1)}(A^r)(V) - \frac{1}{2} D^{(2)}(A^r)(V, V) \right] \\ &= r(r-1)(r-2) \int_0^1 ds \int_0^s d\tau \int_a^b \lambda^{r-3} \operatorname{Tr}[V_1^2 E(\lambda) - V_{1\tau}^2 E_\tau(\lambda)] d\lambda \\ &+ r(r-1)(r-2) \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^b \lambda^{r-3} \eta_{2\tau}^{(n)}(\lambda) d\lambda \\ &= r(r-1)(r-2) \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^b \lambda^{r-3} \eta_\tau^{(n)}(\lambda) d\lambda \\ &= \lim_{n \rightarrow \infty} \int_a^b (\lambda^r)''' \eta^{(n)}(\lambda) d\lambda, \end{aligned}$$

where

$$\eta^{(n)}(\lambda) \equiv \int_0^1 ds \int_0^s d\tau \eta_\tau^{(n)}(\lambda)$$

and

$$\eta_\tau^{(n)}(\lambda) = [\operatorname{Tr}\{V_1^2 E(\lambda) - V_{1\tau}^2 E_\tau(\lambda)\} + \eta_{2\tau}^{(n)}(\lambda)].$$

The interchange of limit and the τ - and s -integrals are justified by an easy application of bounded convergence theorem. Note that $\eta^{(n)}$ is a real-valued function $\forall n$.

Next we want to show that $\{\eta^{(n)}\}$ is Cauchy in $L^1([a, b])$ and we follow the idea from [7]. For that let $f \in L^\infty([a, b])$. Define $g(\lambda) = \int_a^\lambda f(t)dt$ and $h(\lambda) = \int_a^\lambda g(\mu)d\mu$, then $g'(\lambda) = f(\lambda)$ a.e. and $h'(\lambda) = g(\lambda)$. Now consider the expression

$$\begin{aligned} & \int_a^b f(\lambda)[\eta_\tau^{(n)}(\lambda) - \eta_\tau^{(m)}(\lambda)]d\lambda \\ &= \int_a^b f(\lambda)[\eta_{2\tau}^{(n)}(\lambda) - \eta_{2\tau}^{(m)}(\lambda)]d\lambda \\ &= \int_a^b h'(\lambda)d\lambda \left(\int_a^\lambda \text{Tr}(V_{2\tau}[E_\tau(\mu), Y^{(n)} - Y^{(m)}] \right. \\ & \quad \left. - V_2[E(\mu), Y_0^{(n)} - Y_0^{(m)}])d\mu \right), \end{aligned}$$

which on integration by parts twice and on observing that the boundary term for $\lambda = a$ vanishes, leads to

$$\begin{aligned} & h'(b) \int_a^b \text{Tr}(V_{2\tau}[E_\tau(\mu), Y^{(n)} - Y^{(m)}] - V_2[E(\mu), Y_0^{(n)} - Y_0^{(m)}])d\mu \\ & - \left\{ h(\lambda) \text{Tr}(V_{2\tau}[E_\tau(\lambda), Y^{(n)} - Y^{(m)}] - V_2[E(\lambda), Y_0^{(n)} - Y_0^{(m)}]) \Big|_{\lambda=a}^b \right. \\ & \left. - \int_a^b h(\lambda) \text{Tr}(V_{2\tau}[E_\tau(d\lambda), Y^{(n)} - Y^{(m)}] - V_2[E(d\lambda), Y_0^{(n)} - Y_0^{(m)}]) \right\} \\ &= h'(b) \int_a^b \text{Tr}(V_{2\tau}[E_\tau(\mu), Y^{(n)} - Y^{(m)}] - V_2[E(\mu), Y_0^{(n)} - Y_0^{(m)}])d\mu \\ & + \int_a^b h(\lambda) \text{Tr}(V_{2\tau}[E_\tau(d\lambda), Y^{(n)} - Y^{(m)}] - V_2[E(d\lambda), Y_0^{(n)} - Y_0^{(m)}])d\mu. \end{aligned} \tag{2.11}$$

Next we use the identity

$$\begin{aligned} \text{Tr}(V_{2\tau}V_{2\tau}^{(n)} - V_2V_2^{(n)}) &= - \int_a^b \text{Tr}(V_{2\tau}[E_\tau(\mu), Y^{(n)}] \\ & \quad - V_2[E(\mu), Y_0^{(n)}])d\mu \end{aligned}$$

to reduce the above expression in (2.11) to

$$\begin{aligned} & g(b) \text{Tr}(V_2[V_2^{(n)} - V_2^{(m)}] - V_{2\tau}[V_{2\tau}^{(n)} - V_{2\tau}^{(m)}]) \\ & + \text{Tr}(V_{2\tau}[h(A_\tau), Y^{(n)} - Y^{(m)}] - V_2[h(A), Y_0^{(n)} - Y_0^{(m)}]). \end{aligned} \tag{2.12}$$

But on the other hand,

$$[h(A), Y_0^{(n)}] = \int_a^b \int_a^b \frac{h(\lambda) - h(\mu)}{\lambda - \mu} E(d\lambda) V_2^{(n)} E(d\mu)$$

and

$$\begin{aligned} & \text{Tr}(V_2[h(A), Y_0^{(n)} - Y_0^{(m)}]) \\ &= \int_a^b \int_a^b \frac{h(\lambda) - h(\mu)}{\lambda - \mu} \text{Tr}(V_2 E(d\lambda)[V_2^{(n)} - V_2^{(m)}] E(d\mu)) \end{aligned} \tag{2.13}$$

and hence as in [3,4] and in [5],

$$\begin{aligned} |\text{Tr}(V_2[h(A), Y_0^{(n)} - Y_0^{(m)}])| &\leq \|h\|_{\text{Lip}} \|V_2\|_2 \| [V_2^{(n)} - V_2^{(m)}] \|_2 \\ &\leq (b - a) \|f\|_\infty \|V\|_2 \| [V_2^{(n)} - V_2^{(m)}] \|_2 \end{aligned}$$

and hence

$$\begin{aligned} & \sup_{f \in L^\infty([a,b])} \frac{|\int_a^b f(\lambda) [\eta_\tau^{(n)}(\lambda) - \eta_\tau^{(m)}(\lambda)] d\lambda|}{\|f\|_\infty} \\ &\leq 2(b - a) \|V\|_2 (\| [V_2^{(n)} - V_2^{(m)}] \|_2 + \| [V_{2\tau}^{(n)} - V_{2\tau}^{(m)}] \|_2) \end{aligned}$$

i.e. $\|\eta_\tau^{(n)} - \eta_\tau^{(m)}\|_{L^1} \leq 2(b - a) \|V\|_2 (\| [V_2^{(n)} - V_2^{(m)}] \|_2 + \| [V_{2\tau}^{(n)} - V_{2\tau}^{(m)}] \|_2)$, which converges to 0 as $n, m \rightarrow \infty$ and $\forall \tau \in [0, 1]$. A similar computation also shows that $\|\eta_\tau^{(n)}\|_{L^1} \leq 2(b - a) \|V\|_2^2$. Therefore $\{\int_0^1 ds \int_0^s d\tau \eta_\tau^{(n)}(\lambda) \equiv \eta^{(n)}(\lambda)\}$ is also Cauchy in $L^1([a, b])$ and thus there exists a function $\eta \in L^1([a, b])$ such that $\|\eta^{(n)} - \eta\|_{L^1} \rightarrow 0$ as $n \rightarrow \infty$, by the bounded convergence theorem and hence also $\|\eta\|_{L^1} \leq (b - a) \|V\|_2^2$. Therefore,

$$\lim_{n \rightarrow \infty} \int_a^b \lambda^{r-3} \eta^{(n)}(\lambda) d\lambda = \int_a^b \lambda^{r-3} \eta(\lambda) d\lambda$$

and hence

$$\begin{aligned} & \text{Tr} \left[(A + V)^r - A^r - D^{(1)}(A^r)(V) - \frac{1}{2} D^{(2)}(A^r)(V, V) \right] \\ &= r(r - 1)(r - 2) \int_a^b \lambda^{r-3} \eta(\lambda) d\lambda. \end{aligned}$$

For uniqueness, let us assume that there exists $\eta_1, \eta_2 \in L^1([a, b])$ such that

$$\begin{aligned} & \text{Tr} \left[p(A + V) - p(A) - D^{(1)} p(A)(V) - \frac{1}{2} D^{(2)} p(A)(V, V) \right] \\ &= \int_a^b p'''(\lambda) \eta_j(\lambda) d\lambda, \end{aligned}$$

where $p(\cdot)$ is a polynomial and $j = 1, 2$. Therefore

$$\int_a^b p'''(\lambda) \eta(\lambda) d\lambda = 0 \quad \forall \text{ polynomials } p(\cdot) \quad \text{and} \quad \eta \equiv \eta_1 - \eta_2 \in L^1([a, b]),$$

which together with the fact that $\int_a^b \eta_1(\lambda) d\lambda = \int_a^b \eta_2(\lambda) d\lambda = \frac{1}{6} \text{Tr}(V^3)$ (which one can easily arrive at by setting $p(\lambda) = \lambda^3$ in the above formula), implies that $\int_a^b \lambda^r \eta(\lambda) d\lambda = 0 \quad \forall r \geq 0$. Hence by an application of Fubini's theorem, we get that

$$\int_{-\infty}^{\infty} e^{-it\lambda} \eta(\lambda) d\lambda = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{-\infty}^{\infty} (-it\lambda)^n \eta(\lambda) d\lambda = 0.$$

Hence

$$\int_{-\infty}^{\infty} e^{-it\lambda} \eta(\lambda) d\lambda = 0 \quad \forall t \in \mathbb{R}.$$

Therefore η is an $L^1([a, b])$ -function whose Fourier transform $\hat{\eta}(t)$ vanishes identically, implying that $\eta = 0$ or $\eta_1 = \eta_2$ a.e. \square

COROLLARY 2.8

Let A and V be two bounded self-adjoint operators in an infinite dimensional Hilbert space \mathcal{H} such that $V \in \mathcal{B}_2(\mathcal{H})$. Then the function $\eta \in L^1([a, b])$ obtained as in Theorem 2.6 satisfies the following equation:

$$\begin{aligned} \int_a^b f(\lambda) \eta(\lambda) d\lambda &= \int_0^1 ds \int_0^s d\tau \int_a^b \int_a^b \frac{h(\lambda) - h(\mu)}{\lambda - \mu} \\ &\quad \times \text{Tr} [V E_\tau(d\lambda) V E_\tau(d\mu) - V E(d\lambda) V E(d\mu)], \end{aligned}$$

where $f(\lambda)$, $g(\lambda)$ and $h(\lambda)$ are as in the proof of the Theorem 2.6.

Proof. By Fubini's theorem we have that

$$\begin{aligned} \int_a^b f(\lambda) \eta^{(n)}(\lambda) d\lambda &= \int_0^1 ds \int_0^s d\tau \int_a^b f(\lambda) \\ &\quad \times [\text{Tr}\{V_1^2 E(\lambda) - V_{1\tau}^2 E_\tau(\lambda)\} + \eta_{2\tau}^{(n)}(\lambda)] d\lambda. \end{aligned}$$

But

$$\begin{aligned} & \int_a^b f(\lambda) \text{Tr}\{V_1^2 E(\lambda) - V_{1\tau}^2 E_\tau(\lambda)\} d\lambda \\ &= \int_a^b g'(\lambda) \text{Tr}[V_1^2 E(\lambda) - V_{1\tau}^2 E_\tau(\lambda)] d\lambda, \end{aligned}$$

which by integrating by parts leads to

$$\begin{aligned}
& g(b) \operatorname{Tr}[V_1^2 - V_{1\tau}^2] + \int_a^b g(\lambda) \operatorname{Tr}[V_{1\tau}^2 E_\tau(d\lambda) - V_1^2 E(d\lambda)] \\
&= g(b) \operatorname{Tr}[V_1^2 - V_{1\tau}^2] + \operatorname{Tr}[V_{1\tau}^2 h'(A_\tau) - V_1^2 h'(A)] \\
&= g(b) \operatorname{Tr}[V_1^2 - V_{1\tau}^2] + \int_a^b \int_a^b \frac{h(\lambda) - h(\mu)}{\lambda - \mu} \\
&\quad \times \operatorname{Tr}[V_{1\tau} E_\tau(d\lambda) V_{1\tau} E_\tau(d\mu) - V_1 E(d\lambda) V_1 E(d\mu)]. \tag{2.14}
\end{aligned}$$

Again by repeating the above calculations to get (2.12) and (2.13) as in the proof of the Theorem 2.6, we conclude that

$$\begin{aligned}
\int_a^b f(\lambda) \eta_{2\tau}^{(n)}(\lambda) d\lambda &= g(b) \operatorname{Tr}[V_2 V_2^{(n)} - V_{2\tau} V_{2\tau}^{(n)}] \\
&\quad + \int_a^b \int_a^b \frac{h(\lambda) - h(\mu)}{\lambda - \mu} \\
&\quad \times \operatorname{Tr}[V_{2\tau} E_\tau(d\lambda) V_{2\tau}^{(n)} E_\tau(d\mu) - V_2 E(d\lambda) V_2^{(n)} E(d\mu)]. \tag{2.15}
\end{aligned}$$

Combining (2.14) and (2.15) we have

$$\begin{aligned}
& \int_a^b f(\lambda) \eta^{(n)}(\lambda) d\lambda \\
&= \int_0^1 ds \int_0^s d\tau g(b) \operatorname{Tr}[(V_1^2 + V_2 V_2^{(n)}) - (V_{2\tau}^2 + V_{2\tau} V_{2\tau}^{(n)})] \\
&\quad + \int_0^1 ds \int_0^s d\tau \int_a^b \int_a^b \frac{h(\lambda) - h(\mu)}{\lambda - \mu} \\
&\quad \times \operatorname{Tr}[V E_\tau(d\lambda)(V_{1\tau} \oplus V_{2\tau}^{(n)}) E_\tau(d\mu) - V E(d\lambda)(V_1 \oplus V_2^{(n)}) E(d\mu)]. \tag{2.16}
\end{aligned}$$

But by definition $V_2^{(n)}$, $V_{2\tau}^{(n)}$ converges to V_2 , $V_{2\tau}$ respectively in $\|\cdot\|_2$ and we have already proved that $\eta^{(n)}$ converges to η in $L^1([a, b])$. Hence by taking limit on both sides of (2.16) we get that

$$\begin{aligned}
\int_a^b f(\lambda) \eta(\lambda) d\lambda &= \int_0^1 ds \int_0^s d\tau \int_a^b \int_a^b \frac{h(\lambda) - h(\mu)}{\lambda - \mu} \\
&\quad \times \operatorname{Tr}[V E_\tau(d\lambda) V E_\tau(d\mu) - V E(d\lambda) V E(d\mu)]. \tag{2.17}
\end{aligned}$$

In the right-hand side of (2.17) we have used the fact that

$$\operatorname{Var}(\mathcal{G}_2^{(n)} - \mathcal{G}_2) \leq \|V\|_2 (\|V_{2\tau}^{(n)} - V_{2\tau}\|_2 + \|V_2 - V_2^{(n)}\|) \longrightarrow 0 \text{ as } n \longrightarrow \infty,$$

where $\mathcal{G}_2^{(n)}(\Delta \times \delta) = \text{Tr}[VE_\tau(\Delta)(V_{1\tau} \oplus V_{2\tau}^{(n)})E_\tau(\delta) - VE(\Delta)(V_1 \oplus V_2^{(n)})E(\delta)]$ and $\mathcal{G}_2(\Delta \times \delta) = \text{Tr}[VE_\tau(\Delta)VE_\tau(\delta) - VE(\Delta)VE(\delta)]$ are complex measures on \mathbb{R}^2 and $\text{Var}(\mathcal{G}_2^{(n)} - \mathcal{G}_2)$ is the variation of $(\mathcal{G}_2^{(n)} - \mathcal{G}_2)$ and also that $\|h\|_{\text{Lip}} \leq (b-a)\|f\|_\infty$. \square

3. Unbounded case

Theorem 3.1. *Let A be an unbounded self-adjoint operator in a Hilbert space \mathcal{H} and let $\phi : \mathbb{R} \rightarrow \mathbb{C}$ be such that $\int_{-\infty}^{\infty} |\hat{\phi}(t)| (1+|t|)^3 dt < \infty$, where $\hat{\phi}$ is the Fourier transform of ϕ . Then $\phi(A)$, $D^{(1)}\phi(A)$, $D^{(2)}\phi(A)$ exist and*

$$[D^{(1)}\phi(A)](X) = i \int_{-\infty}^{\infty} \hat{\phi}(t) dt \int_0^t d\beta e^{i\beta A} X e^{i(t-\beta)A}$$

and

$$\begin{aligned} [D^{(2)}\phi(A)](X, Y) &= i^2 \int_{-\infty}^{\infty} \hat{\phi}(t) dt \int_0^t d\beta \left\{ \int_0^\beta dv e^{ivA} X e^{i(\beta-v)A} Y e^{i(t-\beta)A} \right. \\ &\quad \left. + \int_0^{t-\beta} dv e^{i\beta A} Y e^{ivA} X e^{i(t-\beta-v)A} \right\}, \end{aligned}$$

where $X, Y \in \mathcal{B}_2(\mathcal{H})$.

Proof. That $\phi(A)$ and the expressions on the right-hand side above exist in $\mathcal{B}(\mathcal{H})$ are consequences of the functional calculus and the assumption on $\hat{\phi}$. Next

$$\begin{aligned} \phi(A+X) - \phi(A) &= \int_{-\infty}^{\infty} \hat{\phi}(t) [e^{it(A+X)} - e^{itA}] dt \\ &= \int_{-\infty}^{\infty} \hat{\phi}(t) dt \int_0^t d\beta e^{i\beta(A+X)} i X e^{i(t-\beta)A}. \end{aligned}$$

Therefore

$$\begin{aligned} \phi(A+X) - \phi(A) - i \int_{-\infty}^{\infty} \hat{\phi}(t) dt \int_0^t d\beta e^{i\beta A} X e^{i(t-\beta)A} \\ = i \int_{-\infty}^{\infty} \hat{\phi}(t) dt \int_0^t d\beta [e^{i\beta(A+X)} X e^{i(t-\beta)A} - e^{i\beta A} X e^{i(t-\beta)A}]. \end{aligned}$$

Using the interpolation inequality

$$\|e^{i\beta(A+X)} - e^{i\beta A}\| \leq 2^{(1-\epsilon)} (\|\beta\| \|X\|)^\epsilon \quad (0 \leq \epsilon \leq 1),$$

we get that

$$\begin{aligned} \left\| \phi(A+X) - \phi(A) - i \int_{-\infty}^{\infty} \hat{\phi}(t) dt \int_0^t d\beta e^{i\beta A} X e^{i(t-\beta)A} \right\| \\ \leq \left(\frac{2^{(1-\epsilon)}}{\epsilon+1} \right) \|X\|^{\epsilon+1} \int_{-\infty}^{\infty} |\hat{\phi}(t)| (1+|t|)^{\epsilon+2} dt, \end{aligned}$$

which by virtue of the assumption on $\hat{\phi}$ implies that $D^{(1)}\phi(A)$ exists and that

$$[D^{(1)}\phi(A)](X) = i \int_{-\infty}^{\infty} \hat{\phi}(t) dt \int_0^t d\beta e^{i\beta A} X e^{i(t-\beta)A}.$$

Similarly for $X, Y \in \mathcal{B}(\mathcal{H})$,

$$\begin{aligned} & [D^{(1)}\phi(A+X)](Y) - [D^{(1)}\phi(A)](Y) \\ &= i^2 \int_{-\infty}^{\infty} \hat{\phi}(t) dt \int_0^t d\beta \left\{ \int_0^\beta d\nu e^{i\nu(A+X)} X e^{i(\beta-\nu)A} Y e^{i(t-\beta)(A+X)} \right. \\ & \quad \left. + \int_0^{t-\beta} d\nu e^{i\beta A} Y e^{i\nu(A+X)} X e^{i(t-\beta-\nu)A} \right\} \end{aligned}$$

and one can verify as before that

$$\begin{aligned} & \left\| [D^{(1)}\phi(A+X)](Y) - [D^{(1)}\phi(A)](Y) \right. \\ & \quad - i^2 \int_{-\infty}^{\infty} \hat{\phi}(t) dt \int_0^t d\beta \left\{ \int_0^\beta d\nu e^{i\nu A} X e^{i(\beta-\nu)A} Y e^{i(t-\beta)A} \right. \\ & \quad \left. \left. + \int_0^{t-\beta} d\nu e^{i\beta A} Y e^{i\nu A} X e^{i(t-\beta-\nu)A} \right\} \right\| \\ & \leq K \|X\|^{\epsilon+1} \|Y\| \int_{-\infty}^{\infty} |\hat{\phi}(t)| (1+|t|)^{\epsilon+2} dt \end{aligned}$$

(for some $\epsilon > 0$ and some constant $K \equiv K(\epsilon)$), proving the expression for $[D^{(2)}\phi(A)](X, Y)$. \square

Theorem 3.2. *Let A be an unbounded self-adjoint operator in a Hilbert space \mathcal{H} , V be a self-adjoint operator such that $V \in \mathcal{B}_3(\mathcal{H})$ and furthermore let $\phi \in \mathcal{S}(\mathbb{R})$ (the Schwartz class of smooth functions of rapid decrease). Then*

$$\phi(A+V) - \phi(A) - [D^{(1)}\phi(A)](V) - \frac{1}{2}[D^{(2)}\phi(A)](V, V) \in \mathcal{B}_1(\mathcal{H})$$

and

$$\begin{aligned} & \text{Tr} \left[\phi(A+V) - \phi(A) - [D^{(1)}\phi(A)](V) - \frac{1}{2}[D^{(2)}\phi(A)](V, V) \right] \\ &= \int_{-\infty}^{\infty} i^2 t \hat{\phi}(t) dt \int_0^t d\nu \int_0^1 ds \int_0^s d\tau \\ & \quad \times \text{Tr} [V e^{i(t-\nu)A_\tau} V e^{i\nu A_\tau} - V e^{i(t-\nu)A} V e^{i\nu A}], \end{aligned}$$

where $A_\tau = A + \tau V$ and $0 \leq \tau \leq 1$.

Proof. Since $[0, 1] \ni s \rightarrow e^{itA_s}$ is $\mathcal{B}_3(\mathcal{H})$ -continuously differentiable, uniformly in t ,

$$\begin{aligned}
& \phi(A + V) - \phi(A) - [D^{(1)}\phi(A)](V) \\
&= \int_{-\infty}^{\infty} \hat{\phi}(t) dt [e^{it(A+V)} - e^{itA}] - [D^{(1)}\phi(A)](V) \\
&= \int_{-\infty}^{\infty} \hat{\phi}(t) dt \int_0^1 ds \frac{d}{ds}(e^{itA_s}) - i \int_{-\infty}^{\infty} \hat{\phi}(t) dt \int_0^{\infty} d\beta e^{i\beta A} V e^{i(t-\beta)A} \\
&= \int_{-\infty}^{\infty} \hat{\phi}(t) dt \left[\int_0^1 ds \int_0^t d\beta e^{i\beta A_s} i V e^{i(t-\beta)A_s} \right. \\
&\quad \left. - i \int_0^1 ds \int_0^t d\beta e^{i\beta A} V e^{i(t-\beta)A} \right] \\
&= \int_{-\infty}^{\infty} i \hat{\phi}(t) dt \int_0^1 ds \int_0^t d\beta [e^{i\beta A_s} V e^{i(t-\beta)A_s} - e^{i\beta A} V e^{i(t-\beta)A}] \\
&= \int_{-\infty}^{\infty} i \hat{\phi}(t) Q(t) dt, \\
&\text{where } Q(t) \equiv \int_0^1 ds \int_0^t d\beta [e^{i\beta A_s} V e^{i(t-\beta)A_s} - e^{i\beta A} V e^{i(t-\beta)A}]. \quad (3.1)
\end{aligned}$$

As before, $\tau \in [0, 1] \rightarrow e^{i\beta A_\tau} V e^{i(t-\beta)A_\tau} \in \mathcal{B}_3(\mathcal{H})$ is $\mathcal{B}_{\frac{3}{2}}(\mathcal{H})$ -continuously differentiable, uniformly with respect to β . Then

$$\begin{aligned}
Q(t) &= \int_0^1 ds \int_0^t d\beta \int_0^s d\tau \frac{d}{d\tau}(e^{i\beta A_\tau} V e^{i(t-\beta)A_\tau}) \\
&= i \int_0^1 ds \int_0^s d\tau \int_0^t d\beta \left\{ \int_0^\beta d\nu e^{i\nu A_\tau} V e^{i(\beta-\nu)A_\tau} V e^{i(t-\beta)A_\tau} \right. \\
&\quad \left. + \int_0^{t-\beta} d\nu e^{i\beta A_\tau} V e^{i\nu A_\tau} V e^{i(t-\beta-\nu)A_\tau} \right\},
\end{aligned}$$

where Fubini's theorem has been used to interchange the order of integration. Hence

$$\begin{aligned}
& \phi(A + V) - \phi(A) - [D^{(1)}\phi(A)](V) - \frac{1}{2}[D^{(2)}\phi(A)](V, V) \\
&= \int_{-\infty}^{\infty} i^2 \hat{\phi}(t) dt \int_0^1 ds \int_0^s d\tau \int_0^t d\beta \left\{ \int_0^\beta d\nu [e^{i\nu A_\tau} V e^{i(\beta-\nu)A_\tau} V e^{i(t-\beta)A_\tau} \right. \\
&\quad \left. - e^{i\nu A} V e^{i(\beta-\nu)A} V e^{i(t-\beta)A}] + \int_0^{t-\beta} d\nu [e^{i\beta A_\tau} V e^{i\nu A_\tau} V e^{i(t-\beta-\nu)A_\tau} \right. \\
&\quad \left. - e^{i\beta A} V e^{i\nu A} V e^{i(t-\beta-\nu)A}] \right\}. \quad (3.2)
\end{aligned}$$

Though each of the four individual terms in the integral in (3.2) belongs to $\mathcal{B}_{\frac{3}{2}}(\mathcal{H})$, each of the differences in parenthesis $[\cdot]$ belongs to $\mathcal{B}_1(\mathcal{H})$, e.g.

$$\begin{aligned} & [e^{ivA\tau} V e^{i(\beta-v)A\tau} V e^{i(t-\beta)A\tau} - e^{ivA} V e^{i(\beta-v)A} V e^{i(t-\beta)A}] \\ &= [e^{ivA\tau} - e^{ivA}] V e^{i(\beta-v)A\tau} V e^{i(t-\beta)A\tau} \\ & \quad + e^{ivA} V [e^{i(\beta-v)A\tau} - e^{i(\beta-v)A}] V e^{i(t-\beta)A\tau} \\ & \quad + e^{i(\beta-v)A\tau} V [e^{i(t-\beta)A\tau} - e^{i(t-\beta)A}] \in \mathcal{B}_1(\mathcal{H}), \end{aligned}$$

and its norm $\|[\cdot]\|_1 \leq |\tau| \|V\|_3^3 \{|\nu| + |\beta - \nu| + |t - \beta|\}$, where we have used the estimate $\|e^{ivA\tau} - e^{ivA}\|_3 \leq |\nu\tau| \|V\|_3$. Hence by the hypothesis on $\hat{\phi}$,

$$\phi(A + V) - \phi(A) - [D^{(1)}\phi(A)](V) - \frac{1}{2}[D^{(2)}\phi(A)](V, V) \in \mathcal{B}_1(\mathcal{H})$$

and

$$\begin{aligned} \mathcal{Z} &\equiv \text{Tr} \left[\phi(A + V) - \phi(A) - [D^{(1)}\phi(A)](V) - \frac{1}{2}[D^{(2)}\phi(A)](V, V) \right] \\ &= \int_{-\infty}^{\infty} i^2 \hat{\phi}(t) dt \int_0^1 ds \int_0^s d\tau \int_0^t d\beta \left\{ \int_0^\beta d\nu \right. \\ & \quad \times \text{Tr} [e^{ivA\tau} V e^{i(\beta-v)A\tau} V e^{i(t-\beta)A\tau} - e^{ivA} V e^{i(\beta-v)A} V e^{i(t-\beta)A}] \\ & \quad \left. + \int_0^{t-\beta} d\nu \text{Tr} [e^{i\beta A\tau} V e^{ivA\tau} V e^{i(t-\beta-\nu)A\tau} - e^{i\beta A} V e^{ivA} V e^{i(t-\beta-\nu)A}] \right\}. \end{aligned} \tag{3.3}$$

Again by the cyclicity of trace and a change of variable, the first integral in $\{\cdot\}$ in (3.3) is equal to

$$\begin{aligned} & \int_0^\beta d\nu \text{Tr} [e^{i(t-\beta+\nu)A\tau} V e^{i(\beta-\nu)A\tau} V - e^{i(t-\beta+\nu)A} V e^{i(\beta-\nu)A} V] \\ &= \int_0^\beta d\nu \text{Tr} [V e^{i(t-\nu)A\tau} V e^{ivA\tau} - V e^{i(t-\nu)A} V e^{ivA}]. \end{aligned} \tag{3.4}$$

Similarly, the second integral in $\{\cdot\}$ in (3.3) is equal to

$$\int_0^{t-\beta} d\nu \text{Tr} [V e^{i(t-\nu)A\tau} V e^{ivA\tau} - V e^{i(t-\nu)A} V e^{ivA}]. \tag{3.5}$$

Combining (3.4) and (3.5), we conclude that

$$\begin{aligned} \mathcal{Z} &= \int_{-\infty}^{\infty} i^2 \hat{\phi}(t) dt \int_0^1 ds \int_0^s d\tau \int_0^t d\beta \left\{ \int_0^\beta d\nu \right. \\ & \quad \times \text{Tr} [V e^{i(t-\nu)A\tau} V e^{ivA\tau} - V e^{i(t-\nu)A} V e^{ivA}] \\ & \quad \left. + \int_0^{t-\beta} d\nu \text{Tr} [V e^{i(t-\nu)A\tau} V e^{ivA\tau} - V e^{i(t-\nu)A} V e^{ivA}] \right\}. \end{aligned} \tag{3.6}$$

By a change of variable and the cyclicity of trace, we get that

$$\begin{aligned} & t \int_0^t dv \operatorname{Tr}[V e^{i(t-v)A_\tau} V e^{ivA_\tau} - V e^{i(t-v)A} V e^{ivA}] \\ &= \int_0^t d\beta \left\{ \int_0^\beta dv \operatorname{Tr}[V e^{i(t-v)A_\tau} V e^{ivA_\tau} - V e^{i(t-v)A} V e^{ivA}] \right. \\ & \quad \left. + \int_0^{t-\beta} dv \operatorname{Tr}[V e^{i(t-v)A_\tau} V e^{ivA_\tau} - V e^{i(t-v)A} V e^{ivA}] \right\}, \end{aligned}$$

using which in (3.6) we are lead to the equation

$$\begin{aligned} \mathcal{Z} &= \int_{-\infty}^{\infty} i^2 t \hat{\phi}(t) dt \int_0^t dv \int_0^1 ds \int_0^s d\tau \\ & \quad \times \operatorname{Tr}[V e^{i(t-v)A_\tau} V e^{ivA_\tau} - V e^{i(t-v)A} V e^{ivA}], \end{aligned} \quad (3.7)$$

by an application of Fubini's theorem. \square

Theorem 3.3. *Let A be an unbounded self-adjoint operator in a Hilbert space \mathcal{H} with $\sigma(A) \subseteq [b, \infty)$ for some $b \in \mathbb{R}$ and V be a self-adjoint operator such that $V \in \mathcal{B}_2(\mathcal{H})$. Then there exists a unique real-valued function $\eta \in L^1\left(\mathbb{R}, \frac{d\lambda}{(1+\lambda^2)^{1+\epsilon}}\right)$ (for some $\epsilon > 0$) such that for every $\phi \in \mathcal{S}(\mathbb{R})$ (the Schwartz class of smooth functions of rapid decrease)*

$$\begin{aligned} & \operatorname{Tr} \left[\phi(A+V) - \phi(A) - [D^{(1)}\phi(A)](V) - \frac{1}{2}[D^{(2)}\phi(A)](V, V) \right] \\ &= \int_{-\infty}^{\infty} \phi'''(\lambda) \eta(\lambda) d\lambda. \end{aligned}$$

Proof. Equation (3.7), after an application of Fubini's theorem, yields

$$\begin{aligned} \mathcal{Z} &\equiv \operatorname{Tr} \left[\phi(A+V) - \phi(A) - [D^{(1)}\phi(A)](V) - \frac{1}{2}[D^{(2)}\phi(A)](V, V) \right] \\ &= \int_0^1 ds \int_0^s d\tau \int_{-\infty}^{\infty} i^2 t \hat{\phi}(t) dt \int_0^t dv \\ & \quad \times \operatorname{Tr}[V e^{i(t-v)A_\tau} V e^{ivA_\tau} - V e^{i(t-v)A} V e^{ivA}]. \end{aligned} \quad (3.8)$$

Now

$$\begin{aligned} & \int_0^t dv \operatorname{Tr}[V e^{i(t-v)A_\tau} V e^{ivA_\tau} - V e^{i(t-v)A} V e^{ivA}] \\ &= \int_0^t dv \int_a^\infty \int_a^\infty e^{i(t-v)\lambda} e^{iv\mu} \operatorname{Tr}[V E_\tau(d\lambda) V E_\tau(d\mu) \\ & \quad - V E(d\lambda) V E(d\mu)], \end{aligned} \quad (3.9)$$

where $a = \min\{b, \inf \sigma(A_\tau) [0 < \tau \leq 1]\}$ and $E_\tau(\cdot)$ and $E(\cdot)$ are the spectral families of the operators A_τ and A respectively and the measure $\mathcal{G} : \Delta \times \delta \subseteq \text{Borel}(\mathbb{R}^2) \longrightarrow$

$\text{Tr}[VE_\tau(\Delta)VE_\tau(\delta) - VE(\Delta)VE(\delta)]$ is a complex measure with total variation $\leq 2\|V\|_2^2$ and hence by Fubini's theorem the right-hand side expression in (3.8) is equal to

$$\begin{aligned} & \int_0^1 ds \int_0^s d\tau \int_{-\infty}^\infty i^2 t \hat{\phi}(t) dt \int_a^\infty \int_a^\infty \int_0^t dv e^{i(t-v)\lambda} e^{iv\mu} \\ & \times \text{Tr}[VE_\tau(d\lambda)VE_\tau(d\mu) - VE(d\lambda)VE(d\mu)] \\ & = \int_0^1 ds \int_0^s d\tau \int_{-\infty}^\infty i^2 t \hat{\phi}(t) dt \int_a^\infty \int_a^\infty \frac{e^{it\lambda} - e^{it\mu}}{i(\lambda - \mu)} \\ & \times \text{Tr}[VE_\tau(d\lambda)VE_\tau(d\mu) - VE(d\lambda)VE(d\mu)] \\ & = \int_0^1 ds \int_0^s d\tau \int_{-\infty}^\infty i^2 t \hat{\phi}(t) dt \int_a^\infty t e^{it\lambda} \\ & \times \text{Tr}[V_{1\tau}^2 E_\tau(d\lambda) - V_1^2 E(d\lambda)] \\ & + \int_0^1 ds \int_0^s d\tau \int_{-\infty}^\infty i^2 t \hat{\phi}(t) dt \int_a^\infty \int_a^\infty \frac{e^{it\lambda} - e^{it\mu}}{i(\lambda - \mu)} \\ & \times \text{Tr}[V_{2\tau} E_\tau(d\lambda)V_{2\tau} E_\tau(d\mu) - V_2 E(d\lambda)V_2 E(d\mu)], \end{aligned} \tag{3.10}$$

where we have set $V = V_1 \oplus V_2 = V_{1\tau} \oplus V_{2\tau} \in \mathcal{B}_2(\mathcal{H})$ as in Lemma 2.4 vi(b). Applying Fubini's theorem in the first expression in the right hand side of (3.10), we conclude that

$$\begin{aligned} & \int_0^1 ds \int_0^s d\tau \int_{-\infty}^\infty i^2 t \hat{\phi}(t) dt \int_a^\infty t e^{it\lambda} \text{Tr}[V_{1\tau}^2 E_\tau(d\lambda) - V_1^2 E(d\lambda)] \\ & = \int_0^1 ds \int_0^s d\tau \int_a^\infty \phi''(\lambda) \text{Tr}[V_{1\tau}^2 E_\tau(d\lambda) - V_1^2 E(d\lambda)] \\ & = \int_0^1 ds \int_0^s d\tau \int_a^\infty \phi'''(\lambda) \text{Tr}[V_1^2 E(\lambda) - V_{1\tau}^2 E_\tau(\lambda)] d\lambda, \end{aligned}$$

where we have integrated by parts and observed that the boundary term vanishes. Thus the first term in (3.10) is equal to

$$\begin{aligned} & \int_0^1 ds \int_0^s d\tau \int_a^\infty \phi'''(\lambda) \eta_{1\tau}(\lambda) d\lambda, \\ & \text{where } \eta_{1\tau}(\lambda) = \text{Tr}[V_1^2 E(\lambda) - V_{1\tau}^2 E_\tau(\lambda)]. \end{aligned} \tag{3.11}$$

Now consider the second expression in the right-hand side of (3.10):

$$\begin{aligned} & \int_0^1 ds \int_0^s d\tau \int_{-\infty}^\infty i^2 t \hat{\phi}(t) dt \int_a^\infty \int_a^\infty \frac{e^{it\lambda} - e^{it\mu}}{i(\lambda - \mu)} \\ & \times \text{Tr}[V_{2\tau} E_\tau(d\lambda)V_{2\tau} E_\tau(d\mu) - V_2 E(d\lambda)V_2 E(d\mu)]. \end{aligned} \tag{3.12}$$

Since $V_{2\tau} \in [\text{Ker}(\mathcal{M}_{(A_\tau+i)^{-1}})]^\perp = \overline{\text{Ran}(\mathcal{M}_{(A_\tau+i)^{-1}}^*)} = \overline{\text{Ran}(\mathcal{M}_{(A_\tau-i)^{-1})}$, there exists a sequence $\{V_{2\tau}^{(n)}\} \subseteq \text{Ran}(\mathcal{M}_{(A_\tau-i)^{-1})}$ i.e. $V_{2\tau}^{(n)} = (A_\tau - i)^{-1} Y^{(n)} -$

$Y^{(n)}(A_\tau - i)^{-1}$ for some $Y^{(n)} \in \mathcal{B}_2(\mathcal{H})$ such that $V_{2\tau}^{(n)} \rightarrow V_{2\tau}$ in $\|\cdot\|_2$. Similarly, there exists a sequence $\{V_2^{(n)}\} \subseteq \text{Ran}(\mathcal{M}_{(A-i)^{-1}})$ i.e. $V_2^{(n)} = (A - i)^{-1} Y_0^{(n)} - Y_0^{(n)}(A - i)^{-1}$ for $Y_0^{(n)} \in \mathcal{B}_2(\mathcal{H})$ such that $V_2^{(n)} \rightarrow V_2$ in $\|\cdot\|_2$. Furthermore, it is easy to see that $\tau \rightarrow (A + \tau V + i)^{-1}$ is holomorphic and therefore by Lemma 2.4 (vii)(b), the map $[0, 1] \ni \tau \rightarrow V_{1\tau}, V_{2\tau}$ are continuous. Thus the expression in (3.12) is equal to

$$\begin{aligned} & \int_0^1 ds \int_0^s d\tau \int_{-\infty}^{\infty} i^2 t \hat{\phi}(t) dt \int_a^{\infty} \int_a^{\infty} \frac{e^{it\lambda} - e^{it\mu}}{i(\lambda - \mu)} \lim_{n \rightarrow \infty} \\ & \times \text{Tr}[V_{2\tau} E_\tau(d\lambda) V_{2\tau}^{(n)} E_\tau(d\mu) - V_2 E(d\lambda) V_2^{(n)} E(d\mu)] \\ & = \int_0^1 ds \int_0^s d\tau \int_{-\infty}^{\infty} i^2 t \hat{\phi}(t) dt \lim_{n \rightarrow \infty} \int_a^{\infty} \int_a^{\infty} \frac{e^{it\lambda} - e^{it\mu}}{i(\lambda - \mu)} \\ & \times \text{Tr}[V_{2\tau} E_\tau(d\lambda) V_{2\tau}^{(n)} E_\tau(d\mu) - V_2 E(d\lambda) V_2^{(n)} E(d\mu)], \end{aligned} \quad (3.13)$$

since $\text{Var}(\mathcal{G}_2^{(n)} - \mathcal{G}_2) \leq \|V_{2\tau}\|_2 \|V_{2\tau}^{(n)} - V_{2\tau}\|_2 + \|V\|_2 \|V_2 - V_2^{(n)}\| \rightarrow 0$ as $n \rightarrow \infty$, where $\mathcal{G}_2(\Delta \times \delta) = \text{Tr}[V_{2\tau} E_\tau(\Delta) V_{2\tau} E_\tau(\delta) - V_2 E(\Delta) V_2 E(\delta)]$ and $\mathcal{G}_2^{(n)}(\Delta \times \delta)$ is the same expression with second V_2 -terms replaced by $V_2^{(n)}$. These are complex measures on \mathbb{R}^2 and $\text{Var}(\mathcal{G}_2^{(n)} - \mathcal{G}_2)$ is the variation of $(\mathcal{G}_2^{(n)} - \mathcal{G}_2)$. Note that

$$\begin{aligned} & \text{Tr}(V_{2\tau} E_\tau(d\lambda) V_{2\tau}^{(n)} E_\tau(d\mu)) \\ & = \text{Tr}(V_{2\tau} E_\tau(d\lambda) [(A_\tau - i)^{-1} Y^{(n)} - Y^{(n)}(A_\tau - i)^{-1}] E_\tau(d\mu)) \\ & = \frac{-(\lambda - \mu)}{(\lambda - i)(\mu - i)} \text{Tr}(V_{2\tau} E_\tau(d\lambda) Y^{(n)} E_\tau(d\mu)) \end{aligned}$$

and since $\int_{-\infty}^{\infty} |t \hat{\phi}(t)| dt < \infty$ and the other functions are bounded, the right-hand side expression in (3.13) is equal to

$$\begin{aligned} & \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_{-\infty}^{\infty} i^2 t \hat{\phi}(t) dt \int_a^{\infty} \int_a^{\infty} \frac{e^{it\lambda} - e^{it\mu}}{i(\lambda - \mu)} \left[\frac{-(\lambda - \mu)}{(\lambda - i)(\mu - i)} \right] \\ & \times \text{Tr}\{V_{2\tau} E_\tau(d\lambda) Y^{(n)} E_\tau(d\mu) - V_2 E(d\lambda) Y_0^{(n)} E(d\mu)\} \\ & = \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_{-\infty}^{\infty} -it \hat{\phi}(t) dt \int_a^{\infty} \int_a^{\infty} [e^{it\lambda} - e^{it\mu}] \\ & \times \text{Tr}\{V_{2\tau} E_\tau(d\lambda) (A_\tau - i)^{-1} Y^{(n)} (A_\tau - i)^{-1} E_\tau(d\mu) \\ & - V_2 E(d\lambda) (A - i)^{-1} Y_0^{(n)} (A - i)^{-1} E(d\mu)\} \\ & = \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_{-\infty}^{\infty} -it \hat{\phi}(t) dt \int_a^{\infty} e^{it\lambda} \\ & \times \text{Tr}(V_{2\tau}[E_\tau(d\lambda), \tilde{Y}^{(n)}] - V_2[E(d\lambda), \tilde{Y}_0^{(n)}]), \end{aligned} \quad (3.14)$$

where $\tilde{Y}^{(n)} = (A_\tau - i)^{-1} Y^{(n)} (A_\tau - i)^{-1}$ and $\tilde{Y}_0^{(n)} = (A - i)^{-1} Y_0^{(n)} (A - i)^{-1}$. Again by applying Fubini's theorem the right-hand side in (3.14) is equal to

$$\int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^\infty -\phi'(\lambda) \operatorname{Tr}(V_{2\tau}[E_\tau(d\lambda), \tilde{Y}^{(n)}] - V_2[E(d\lambda), \tilde{Y}_0^{(n)}]),$$

and by integrating by parts twice and on observing that the boundary term vanishes, this reduces to

$$\begin{aligned} & \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} - \left\{ \phi'(\lambda) \operatorname{Tr}(V_{2\tau}[E_\tau(\lambda), \tilde{Y}^{(n)}] - V_2[E(\lambda), \tilde{Y}_0^{(n)}]) \Big|_{\lambda=a}^\infty \right. \\ & \quad \left. - \int_a^\infty -\phi''(\lambda) \operatorname{Tr}(V_{2\tau}[E_\tau(\lambda), \tilde{Y}^{(n)}] - V_2[E(\lambda), \tilde{Y}_0^{(n)}]) d\lambda \right\} \\ & = \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^\infty \phi''(\lambda) \\ & \quad \times \operatorname{Tr}(V_{2\tau}[E_\tau(\lambda), \tilde{Y}^{(n)}] - V_2[E(\lambda), \tilde{Y}_0^{(n)}]) d\lambda \\ & = \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \left\{ \phi''(\lambda) \int_a^\lambda \operatorname{Tr}(V_{2\tau}[E_\tau(\mu), \tilde{Y}^{(n)}] \right. \\ & \quad \left. - V_2[E(\mu), \tilde{Y}_0^{(n)}]) d\mu \Big|_{\lambda=a}^\infty \right. \\ & \quad \left. - \int_a^\infty \phi'''(\lambda) \left(\int_a^\lambda \operatorname{Tr}(V_{2\tau}[E_\tau(\mu), \tilde{Y}^{(n)}] \right. \right. \\ & \quad \left. \left. - V_2[E(\mu), \tilde{Y}_0^{(n)}]) d\mu \right) d\lambda \right\} \\ & = \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^\infty \phi'''(\lambda) \\ & \quad \times \left(\int_a^\lambda \operatorname{Tr}(V_2[E(\mu), \tilde{Y}_0^{(n)}] - V_{2\tau}[E_\tau(\mu), \tilde{Y}^{(n)}]) d\mu \right) d\lambda \\ & = \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^\infty \phi'''(\lambda) \eta_{2\tau}^{(n)}(\lambda) d\lambda, \end{aligned} \tag{3.15}$$

where $\eta_{2\tau}^{(n)}(\lambda) = \int_a^\lambda \operatorname{Tr}(V_2[E(\mu), \tilde{Y}_0^{(n)}] - V_{2\tau}[E_\tau(\mu), \tilde{Y}^{(n)}]) d\mu$.

Here it is worth observing that the hypothesis that A is bounded below is used for the first time, only for performing the second integration by parts. Combining (3.11) and (3.15), we conclude that

$$\begin{aligned} & \operatorname{Tr} \left[\phi(A + V) - \phi(A) - [D^{(1)}\phi(A)](V) - \frac{1}{2}[D^{(2)}\phi(A)](V, V) \right] \\ & = \int_0^1 ds \int_0^s d\tau \lim_{n \rightarrow \infty} \int_a^\infty \phi'''(\lambda) \eta_\tau^{(n)}(\lambda) d\lambda, \end{aligned} \tag{3.16}$$

where $\eta_\tau^{(n)}(\lambda) = \eta_{1\tau}(\lambda) + \eta_{2\tau}^{(n)}(\lambda)$. We claim that $\{\eta_\tau^{(n)}\}$ is a Cauchy sequence in $L^1\left(\mathbb{R}, \frac{d\lambda}{(1+\lambda^2)^{1+\epsilon}}\right)$ ($\epsilon > 0$) and we follow the idea from [7]. First note that $L^\infty(\mathbb{R}, d\lambda) = L^\infty(\mathbb{R}, \psi(\lambda)d\lambda)$, where $\psi(\lambda) = \frac{1}{(1+\lambda^2)^{1+\epsilon}}$ since the two measures are equivalent. Next, let $f \in L^\infty(\mathbb{R}, d\lambda)$ and define

$$g(\lambda) = \int_\lambda^\infty f(t)\psi(t)dt \quad \text{for } \lambda \in \mathbb{R}.$$

Then g is absolutely continuous with $g'(\lambda) = -f(\lambda)\psi(\lambda)$ a.e. and that $|g(\lambda)| \leq \text{const.} \frac{1}{(1+\lambda^2)^{\frac{1}{2}+\epsilon'}}$ (for some $\epsilon' > 0$) for $\lambda \rightarrow \infty$ and bounded. Next consider the expression

$$\begin{aligned} & \int_{-\infty}^\infty f(\lambda)\psi(\lambda)[\eta_\tau^{(n)}(\lambda) - \eta_\tau^{(m)}(\lambda)]d\lambda \\ &= \int_a^\infty f(\lambda)\psi(\lambda)[\eta_{2\tau}^{(n)}(\lambda) - \eta_{2\tau}^{(m)}(\lambda)]d\lambda \\ &= \int_a^\infty -g'(\lambda) d\lambda \left(\int_a^\lambda \text{Tr}(V_2[E(\mu), \tilde{Y}_0^{(n)} - \tilde{Y}_0^{(m)}] \right. \\ & \quad \left. - V_{2\tau}[E_\tau(\mu), \tilde{Y}^{(n)} - \tilde{Y}^{(m)}])d\mu \right), \end{aligned}$$

which on integration by parts and on observing that the boundary term vanishes, leads to

$$\int_a^\infty g(\lambda)\text{Tr}(V_2[E(\lambda), \tilde{Y}_0^{(n)} - \tilde{Y}_0^{(m)}] - V_{2\tau}[E_\tau(\lambda), \tilde{Y}^{(n)} - \tilde{Y}^{(m)}])d\lambda. \tag{3.17}$$

Define

$$h(\lambda) = \int_a^\lambda g(t)dt \quad \text{for } \lambda \in [a, \infty).$$

Then h is bounded, differentiable on $[a, \infty)$ with $h'(\lambda) = g(\lambda) \forall \lambda \in [a, \infty)$. Hence by integrating by parts and observing that the boundary term vanishes, the right-hand side in (3.17) is equal to

$$\begin{aligned} & \int_a^\infty h'(\lambda)\text{Tr}(V_2[E(\lambda), \tilde{Y}_0^{(n)} - \tilde{Y}_0^{(m)}] - V_{2\tau}[E_\tau(\lambda), \tilde{Y}^{(n)} - \tilde{Y}^{(m)}])d\lambda \\ &= h(\lambda) \text{Tr}(V_2[E(\lambda), \tilde{Y}_0^{(n)} - \tilde{Y}_0^{(m)}] - V_{2\tau}[E_\tau(\lambda), \tilde{Y}^{(n)} - \tilde{Y}^{(m)}]) \Big|_{\lambda=a}^\infty \\ & \quad - \int_a^\infty h(\lambda)\text{Tr}(V_2[E(d\lambda), \tilde{Y}_0^{(n)} - \tilde{Y}_0^{(m)}] \\ & \quad - V_{2\tau}[E_\tau(d\lambda), \tilde{Y}^{(n)} - \tilde{Y}^{(m)}]) \\ &= \int_a^\infty h(\lambda) \text{Tr}(V_{2\tau}[E_\tau(d\lambda), \tilde{Y}^{(n)} - \tilde{Y}^{(m)}] - V_2[E(d\lambda), \tilde{Y}_0^{(n)} - \tilde{Y}_0^{(m)}]) \\ &= \text{Tr}(V_{2\tau}[h(A_\tau), \tilde{Y}^{(n)} - \tilde{Y}^{(m)}] - V_2[h(A), \tilde{Y}_0^{(n)} - \tilde{Y}_0^{(m)}]). \end{aligned} \tag{3.18}$$

But on the other hand,

$$\begin{aligned}
& [h(A), \tilde{Y}_0^{(n)}] \\
&= \int_a^\infty \int_a^\infty [h(\lambda) - h(\mu)] E(d\lambda) \tilde{Y}_0^{(n)} E(d\mu) \\
&= \int_a^\infty \int_a^\infty [h(\lambda) - h(\mu)] (\lambda - i)^{-1} (\mu - i)^{-1} E(d\lambda) Y_0^{(n)} E(d\mu) \\
&= \int_a^\infty \int_a^\infty \frac{h(\lambda) - h(\mu)}{(\lambda - i)^{-1} - (\mu - i)^{-1}} (\lambda - i)^{-1} (\mu - i)^{-1} E(d\lambda) V_2^{(n)} E(d\mu)
\end{aligned}$$

and hence

$$[h(A), \tilde{Y}_0^{(n)}] = - \int_a^\infty \int_a^\infty \frac{h(\lambda) - h(\mu)}{\lambda - \mu} E(d\lambda) V_2^{(n)} E(d\mu).$$

Therefore

$$\begin{aligned}
\text{Tr}(V_2[h(A), \tilde{Y}_0^{(n)} - \tilde{Y}_0^{(m)}]) &= - \int_a^\infty \int_a^\infty \frac{h(\lambda) - h(\mu)}{\lambda - \mu} \\
&\times \text{Tr}(V_2 E(d\lambda) [V_2^{(n)} - V_2^{(m)}] E(d\mu))
\end{aligned} \tag{3.19}$$

and hence as in [3,4] and in [5],

$$|\text{Tr}(V_2[h(A), \tilde{Y}_0^{(n)} - \tilde{Y}_0^{(m)}])| \leq \|f\|_\infty \|\psi\|_{L^1} \|V\|_2 \| [V_2^{(n)} - V_2^{(m)}] \|_2$$

and hence

$$\begin{aligned}
& \sup_{f \in L^\infty(\mathbb{R})} \frac{\left| \int_{-\infty}^\infty f(\lambda) \psi(\lambda) [\eta_\tau^{(n)}(\lambda) - \eta_\tau^{(m)}(\lambda)] d\lambda \right|}{\|f\|_\infty} \\
&\leq \|\psi\|_{L^1} \|V\|_2 (\| [V_2^{(n)} - V_2^{(m)}] \|_2 + \| [V_{2\tau}^{(n)} - V_{2\tau}^{(m)}] \|_2),
\end{aligned}$$

i.e.

$$\begin{aligned}
& \|\eta_\tau^{(n)} - \eta_\tau^{(m)}\|_{L^1(\mathbb{R}, \psi(\lambda) d\lambda)} \\
&\leq \|\psi\|_{L^1} \|V\|_2 (\| [V_2^{(n)} - V_2^{(m)}] \|_2 + \| [V_{2\tau}^{(n)} - V_{2\tau}^{(m)}] \|_2),
\end{aligned}$$

which converges to 0 as $m, n \rightarrow \infty$ and $\forall \tau \in [0, 1]$. A similar computation also shows that $\|\eta_\tau^{(n)}\|_{L^1(\mathbb{R}, \psi(\lambda) d\lambda)} \leq 2\|\psi\|_{L^1} \|V\|_2^2$, independent of τ and n . Therefore $\{\int_0^1 ds \int_0^s d\tau \eta_\tau^{(n)}(\lambda) \equiv \eta^{(n)}(\lambda)\}$ is also Cauchy in $L^1(\mathbb{R}, \psi(\lambda) d\lambda)$ and thus there exists a function $\eta \in L^1(\mathbb{R}, \psi(\lambda) d\lambda)$ such that $\|\eta^{(n)} - \eta\|_{L^1(\mathbb{R}, \psi(\lambda) d\lambda)} \rightarrow 0$ as $n \rightarrow \infty$, by the bounded convergence theorem and also $\|\eta\|_{L^1(\mathbb{R}, \psi(\lambda) d\lambda)} \leq \|\psi\|_{L^1} \|V\|_2^2$. Therefore by

using the dominated convergence theorem as well as Fubini's theorem, from (3.16) we conclude that

$$\begin{aligned} & \text{Tr} \left[\phi(A + V) - \phi(A) - [D^{(1)}\phi(A)](V) - \frac{1}{2}[D^{(2)}\phi(A)](V, V) \right] \\ &= \int_{-\infty}^{\infty} \phi'''(\lambda)\eta(\lambda)d\lambda. \end{aligned}$$

□

The proof of the uniqueness and the real-valued nature of η is postponed till after Corollary 3.4.

COROLLARY 3.4

Let A be an unbounded self-adjoint operator in a Hilbert space \mathcal{H} with $\sigma(A) \subseteq [b, \infty)$ for some $b \in \mathbb{R}$ and V be a self-adjoint operator such that $V \in \mathcal{B}_2(\mathcal{H})$. Then the function $\eta \in L^1(\mathbb{R}, \psi(\lambda)d\lambda)$ obtained as in Theorem 3.3 satisfies the following equation

$$\begin{aligned} & \int_{-\infty}^{\infty} f(\lambda)\psi(\lambda)\eta(\lambda)d\lambda \\ &= \int_0^1 ds \int_0^s d\tau \int_a^\infty \int_a^\infty \frac{h(\lambda) - h(\mu)}{\lambda - \mu} \\ & \quad \times \text{Tr}[V E(d\lambda) V E(d\mu) \\ & \quad - V E_\tau(d\lambda) V E_\tau(d\mu)], \end{aligned} \tag{3.20}$$

where $f(\lambda)$, $g(\lambda)$, $h(\lambda)$ and $\psi(\lambda)$ are as in the proof of Theorem 3.3.

Proof. By Fubini's theorem we have that

$$\begin{aligned} & \int_{-\infty}^{\infty} f(\lambda)\psi(\lambda)\eta^{(n)}(\lambda)d\lambda \\ &= \int_0^1 ds \int_0^s d\tau \int_a^\infty f(\lambda)\psi(\lambda)[\eta_{1\tau}(\lambda) + \eta_{2\tau}^{(n)}(\lambda)]d\lambda. \end{aligned}$$

But

$$\int_a^\infty f(\lambda)\psi(\lambda)\eta_{1\tau}(\lambda)d\lambda = \int_a^\infty -g'(\lambda)\text{Tr}[V_1^2 E(\lambda) - V_{1\tau}^2 E_\tau(\lambda)]d\lambda,$$

which by integrating by parts and observing that the boundary terms vanishes, leads to

$$\int_a^\infty g(\lambda)\text{Tr}[V_1^2 E(d\lambda) - V_{1\tau}^2 E_\tau(d\lambda)] = \text{Tr}[V_1^2 h'(A) - V_{1\tau}^2 h'(A_\tau)],$$

which by Lemma 2.4(ii) is equal to

$$\int_a^\infty \int_a^\infty \frac{h(\lambda) - h(\mu)}{\lambda - \mu} \text{Tr}[V_1 E(d\lambda) V_1 E(d\mu) - V_{1\tau} E_\tau(d\lambda) V_{1\tau} E_\tau(d\mu)]. \tag{3.21}$$

Again by repeating the same calculations as in the proof of Theorem 3.3, we conclude that

$$\begin{aligned}
& \int_a^\infty f(\lambda) \psi(\lambda) \eta_{2\tau}^{(n)}(\lambda) d\lambda \\
&= \int_a^\infty \int_a^\infty \frac{h(\lambda) - h(\mu)}{\lambda - \mu} \\
&\quad \times \text{Tr}[V_2 E(d\lambda) V_2^{(n)} E(d\mu) - V_{2\tau} E_\tau(d\lambda) V_{2\tau}^{(n)} E_\tau(d\mu)]. \tag{3.22}
\end{aligned}$$

Combining (3.21) and (3.22) we have

$$\begin{aligned}
& \int_{-\infty}^\infty f(\lambda) \psi(\lambda) \eta^{(n)}(\lambda) d\lambda \\
&= \int_0^1 ds \int_0^s d\tau \int_a^\infty \int_a^\infty \frac{h(\lambda) - h(\mu)}{\lambda - \mu} \\
&\quad \times \text{Tr}[(V_1 \oplus V_2) E(d\lambda) (V_1 \oplus V_2^{(n)}) E(d\mu) \\
&\quad - (V_{1\tau} \oplus V_{2\tau}) E_\tau(d\lambda) (V_{1\tau} \oplus V_{2\tau}^{(n)}) E_\tau(d\mu)]. \tag{3.23}
\end{aligned}$$

But by definition $V_2^{(n)}$, $V_{2\tau}^{(n)}$ converges to V_2 , $V_{2\tau}$ respectively in $\|\cdot\|_2$ and we have already proved that $\eta^{(n)}$ converges to η in $L^1(\mathbb{R}, \psi(\lambda) d\lambda)$. Hence by taking limit on both sides of (3.23) we get that

$$\begin{aligned}
& \int_{-\infty}^\infty f(\lambda) \psi(\lambda) \eta(\lambda) d\lambda \\
&= \int_0^1 ds \int_0^s d\tau \int_a^\infty \int_a^\infty \frac{h(\lambda) - h(\mu)}{\lambda - \mu} \\
&\quad \times \text{Tr}[V E(d\lambda) V E(d\mu) - V E_\tau(d\lambda) V E_\tau(d\mu)], \tag{3.24}
\end{aligned}$$

where we have used the fact that $\text{Var}(\mathcal{G}_2^{(n)} - \mathcal{G}_2) \leq \|V\|_2 (\|V_{2\tau}^{(n)} - V_{2\tau}\|_2 + \|V_2 - V_{2\tau}^{(n)}\|) \rightarrow 0$, and that $\|h\|_{\text{Lip}} \leq \|g\|_\infty \leq \|f\|_\infty \|\psi\|_{L^1}$. \square

Proof of uniqueness and real-valued property of η . For uniqueness in Theorem 3.3, let us assume that there exists $\eta_1, \eta_2 \in L^1(\mathbb{R}, \psi(\lambda) d\lambda)$ such that

$$\begin{aligned}
& \text{Tr} \left[\phi(A + V) - \phi(A) - [D^{(1)}\phi(A)](V) - \frac{1}{2} [D^{(2)}\phi(A)](V, V) \right] \\
&= \int_{-\infty}^\infty \phi'''(\lambda) \eta_j(\lambda) d\lambda
\end{aligned}$$

for $j = 1, 2$. Then using Corollary 3.4 we conclude that

$$\int_{\mathbb{R}} f(\lambda) \psi(\lambda) \eta_j(\lambda) d\lambda = \int_0^1 ds \int_0^s d\tau \int_a^\infty \int_a^\infty \frac{h(\lambda) - h(\mu)}{\lambda - \mu} \\ \times \text{Tr} [VE(d\lambda)VE(d\mu) - VE_\tau(d\lambda)VE_\tau(d\mu)],$$

for $j = 1, 2$ and for all $f \in L^\infty(\mathbb{R})$. Hence

$$\int_{\mathbb{R}} f(\lambda) \psi(\lambda) \eta(\lambda) d\lambda = 0, \quad \forall f \in L^\infty(\mathbb{R}), \quad (3.25)$$

where $\eta(\lambda) \equiv \eta_1(\lambda) - \eta_2(\lambda) \in L^1(\mathbb{R}, \psi(\lambda)d\lambda)$. Since (3.25) is true for all $f \in L^\infty(\mathbb{R})$, in particular it is true for all real-valued $f \in L^\infty(\mathbb{R})$, i.e.

$$\int_{\mathbb{R}} f(\lambda) \psi(\lambda) \eta(\lambda) d\lambda = 0, \quad \forall \text{ real valued } f \in L^\infty(\mathbb{R}). \quad (3.26)$$

Let $\eta(\lambda) = \eta_{\text{Rel}}(\lambda) + i\eta_{\text{Img}}(\lambda)$, where $\eta_{\text{Rel}}(\lambda)$ and $\eta_{\text{Img}}(\lambda)$ are real valued $L^1(\mathbb{R}, \psi(\lambda)d\lambda)$ -function. Hence from (3.26), we conclude that

$$\int_{\mathbb{R}} f(\lambda) \psi(\lambda) \eta_{\text{Rel}}(\lambda) d\lambda = 0 \\ = \int_{\mathbb{R}} f(\lambda) \psi(\lambda) \eta_{\text{Img}}(\lambda) d\lambda, \quad \forall \text{ real valued } f \in L^\infty(\mathbb{R}). \quad (3.27)$$

In particular if we consider $f(\lambda) = \text{sgn } \eta_{\text{Rel}}(\lambda)$, where $\text{sgn } \eta_{\text{Rel}}(\lambda) = 0, \forall \lambda$ such that $\eta_{\text{Rel}}(\lambda) = 0$; $\text{sgn } \eta_{\text{Rel}}(\lambda) = 1, \forall \lambda$ such that $\eta_{\text{Rel}}(\lambda) > 0$; $\text{sgn } \eta_{\text{Rel}}(\lambda) = -1, \forall \lambda$ such that $\eta_{\text{Rel}}(\lambda) < 0$. Then $f = \text{sgn } \eta_{\text{Rel}} \in L^\infty(\mathbb{R})$ and hence

$$\int_{\mathbb{R}} |\eta_{\text{Rel}}(\lambda)| |\psi(\lambda)| d\lambda = \int_{\mathbb{R}} \text{sgn } \eta_{\text{Rel}}(\lambda) \eta_{\text{Rel}}(\lambda) \psi(\lambda) d\lambda = 0,$$

which implies that $|\eta_{\text{Rel}}(\lambda)| |\psi(\lambda)| = 0$ a.e. and hence $\eta_{\text{Rel}}(\lambda) = 0$ a.e. Similarly by the same above argument we conclude that $\eta_{\text{Img}}(\lambda) = 0$ a.e. and hence $\eta(\lambda) = 0$ a.e. Therefore $\eta_1(\lambda) = \eta_2(\lambda)$ a.e. Again, since the right-hand side of (3.20) is real for all real-valued $f \in L^\infty(\mathbb{R})$, by a similar argument as above, it follows that η is real valued.

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