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MULTIPLE OPERATOR INTEGRALS AND SPECTRAL SHIFT

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ABSTRACT. Multiple scalar integral representations for traces of operator derivatives are obtained and applied in the proof of existence of the higher order spectral shift functions.

1. Introduction

For a large class of admissible functions $f:\mathbb{R}\mapsto\mathbb{C}$, the operator derivatives $\frac{d^j}{dx^j}f(H_0+xV)$, where H_0 and V are self-adjoint operators on a separable Hilbert space $\mathcal{H}$, exist and can be represented as multiple operator integrals [1], [14]. We explore properties of operator derivatives inside a semi-finite normal faithful trace τ given on a semi-finite von Neumann algebra $\mathcal{M}$ acting on $\mathcal{H}$.

For $H_0=H_0^*$ affiliated with $\mathcal{M}$ and $V=V^*$ in the τ-Hilbert–Schmidt class $\mathcal{L}_2(\mathcal{M},\tau)$ (that is, $V\in\mathcal{M}$ and $\tau(|V|^2)<\infty$), we represent the traces of the derivatives $\tau[\frac{d^j}{dx^j}f(H_0+xV)]$ as multiple scalar integrals, and, subsequently, as a distribution on $f^{(j)}$, which is essentially a derivative of an L^∞-function (see Theorem 3.12 and Corollary 3.14). We also obtain that the order of an operator derivative inside the trace can be decreased, which costs the increase of the order of a scalar derivative; more precisely,

$$\tau\left[\frac{d^j}{dx^j}f(H_0+xV)\right]=\tau\left[V\frac{d^{j-1}}{dx^{j-1}}f'(H_0+xV)\right]$$

(see Corollary 3.15). The obtained representations for $\tau[\frac{d^j}{dx^j}f(H_0+xV)]$ are applied in derivation of explicit formulas for the remainders of noncommutative Taylor-type approximations (described below) in Section 4.

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Let $R_p(f) \equiv R_{p,H_0,V}(f)$ denote the remainder of the Taylor-type approximation

$$f(H_0+V) - \sum_{j=0}^{p-1} \frac{1}{j!} \frac{d^j}{dx^j}\bigg|_{x=0} f(H_0+xV)$$

of the value of $f(H_0+V)$ at the perturbed operator H_0+V by data determined by the initial operator H_0. Let $\mathcal{W}_p(\mathbb{R})$ denote the set of functions $f \in C^p(\mathbb{R})$ such that for each $j=0,\dots,p$, the derivative $f^{(j)}$ equals the Fourier transform $\int_{\mathbb{R}} e^{it\lambda}\, d\mu_{f^{(j)}}(\lambda)$ of a finite Borel measure $\mu_{f^{(j)}}$. There exist functions $\xi \equiv \xi_{H_0+V,H_0}$ and $\eta \equiv \eta_{H_0,H_0+V}$, called Krein's and Koplienko's spectral shift functions, respectively, such that when $\tau(|V|) < \infty$,

$$\tau\big[R_1(f)\big] = \int_{\mathbb{R}} f'(t)\xi(t)\, dt \tag{1.1}$$

for $f \in \mathcal{W}_1(\mathbb{R})$ [8] (see also [2], [4], [9], [12]), and when $\tau(|V|^2) < \infty$,

$$\tau\big[R_2(f)\big] = \int_{\mathbb{R}} f''(t)\eta(t)\, dt \tag{1.2}$$

for $f \in \mathcal{W}_2(\mathbb{R})$ [7] (see also [6], [10], [13], [15]).

It was conjectured in [7] that for V in the Schatten p-class, $p \geq 3$, and $\mathcal{M} = \mathcal{B}(\mathcal{H})$ (the algebra of bounded operators on $\mathcal{H}$), there exists a real Borel measure $\nu_p \equiv \nu_{p,H_0,V}$, with the total variation bounded by $\frac{\tau(|V|^p)}{p!}$, such that

$$\tau\big[R_p(f)\big] = \int_{\mathbb{R}} f^{(p)}(t)\, d\nu_p(t) \tag{1.3}$$

for bounded rational functions f. A proof of (1.3) was also suggested in [7], but, unfortunately, it contained a mistake (see [6] for details).

It was proved in [6, Theorem 5.1] that (1.3) holds for $f \in \mathcal{W}_p(\mathbb{R})$ when V is in the Hilbert–Schmidt class and $\mathcal{M} = \mathcal{B}(\mathcal{H})$, with ν_p a real Borel measure whose total variation is bounded by $\frac{\tau(|V|^2)^{p/2}}{p!}$. It was shown in [6] and [16] that ν_p is absolutely continuous for a bounded and unbounded H_0, respectively. Moreover, an explicit formula for the density of ν_p, called the spectral shift function of order p, was derived in [6], [16] (see, e.g., (4.3) of Theorem 4.1). The trace formula (1.3) was also obtained in the case of $\mathcal{M}$ a general semifinite von Neumann algebra and $p=3$ [6, Theorem 5.2], with ν_3 absolutely continuous when H_0 is bounded. When H_0 is unbounded, the trace formula (1.3) with an absolutely continuous measure ν_3 was established in [16] for a set of functions f disjoint from the one assured by the part of [6, Theorem 5.2] for an unbounded H_0 (this discrepancy is explained in Remark 4.4).

The proof of existence of the measure ν_p in [6] relied on iterated operator integration techniques, while the proofs of the absolute continuity of ν_p in [6], [16] on analytic function theory techniques. By utilizing the results on operator derivatives and divided differences of Sections 3 and 2, respectively, we obtain a simple proof of positivity of ν_2 (see Section 3), a more direct, unified, proof of the established trace formula (1.3) and the absolute continuity of ν_p (see Section 4). We also obtain a new representation for the density of ν_p (see (4.2) of Theorem 4.1) and, in the case of a general $\mathcal{M}$ and unbounded H_0, extend (1.3) with an absolutely continuous measure ν_3 to a larger (as compared to [16]) set of functions f (see Theorem 4.3). The "spectral shift" meaning of the density of ν_p is demonstrated on an example of commuting operators in a finite von Neumann algebra in Section 4.

2. Divided differences and splines

In this section, we collect facts on divided differences and splines to be used in the sequel.

Definition 2.1. The divided difference of order p is an operation on functions f of one (real) variable, which we will usually call λ, defined recursively as follows:

$$\Delta^{(0)}_{\lambda_1}(f) := f(\lambda_1),$$

$$\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}(f) := \begin{cases} \frac{\Delta^{(p-1)}_{\lambda_1,\dots,\lambda_{p-1},\lambda_p}(f)-\Delta^{(p-1)}_{\lambda_1,\dots,\lambda_{p-1},\lambda_{p+1}}(f)}{\lambda_p-\lambda_{p+1}} & \text{if } \lambda_p \neq \lambda_{p+1}, \\ \frac{\partial}{\partial t}\big|_{t=\lambda_p}\Delta^{(p-1)}_{\lambda_1,\dots,\lambda_{p-1},t}(f) & \text{if } \lambda_p = \lambda_{p+1}. \end{cases}$$

The following facts are well known.

Proposition 2.2.

(1) (*See* [5, Section 4.7(a)].) $\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}(f)$ *is symmetric in* $\lambda_1, \lambda_2, \dots, \lambda_{p+1}$.

(2) (*See* [5, Section 4.7].) *For f a sufficiently smooth function*,

$$\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}(f) = \sum_{i\in\mathcal{I}} \sum_{j=0}^{m(\lambda_i)-1} c_{ij}(\lambda_1,\dots,\lambda_{p+1}) f^{(j)}(\lambda_i).$$

Here $\mathcal{I}$ is the set of indices i for which λ_i are distinct, *$m(\lambda_i)$ is the multiplicity of λ_i, and $c_{ij}(\lambda_1,\dots,\lambda_{p+1}) \in \mathbb{C}$.*

In particular, *if all points $\lambda_1,\dots,\lambda_{p+1}$ are distinct*, *then*

$$\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}(f) = \sum_{j=1}^{p+1} \frac{f(\lambda_j)}{\prod_{k\in\{1,\dots,p+1\}\setminus\{j\}}(\lambda_j - \lambda_k)}.$$

(3) (*See* [5, Section 4.7].)

$$\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}\big(a_p\lambda^p + a_{p-1}\lambda^{p-1} + \dots + a_1\lambda + a_0\big) = a_p, \quad \textit{where } a_0, a_1, \dots, a_p \in \mathbb{C}.$$

(4) (*See* [5, Theorem 6.2 and Theorem 6.3].) *For $f \in C^p[a,b]$*, *the function*

$$[a,b]^{p+1} \ni (\lambda_1,\dots,\lambda_{p+1}) \mapsto \Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}(f)$$

is continuous.

We will need a more specific version of Proposition 2.2(2).

LEMMA 2.3. *Let $f \in C^1[a,b]$ and $\lambda_1, \dots, \lambda_p$ be distinct points in $[a,b]$. Then for any $i \in \{1, \dots, p\}$,*

$$\Delta^{(p)}_{\lambda_1,\dots,\lambda_p,\lambda_i}(f) = \frac{f'(\lambda_i)}{\prod_{k\in\{1,\dots,p\}\setminus\{i\}}(\lambda_i-\lambda_k)} + \sum_{j\in\{1,\dots,p\}\setminus\{i\}} \frac{1}{(\lambda_i-\lambda_j)^2}\Bigg(\frac{f(\lambda_j)}{\prod_{k\in\{1,\dots,p\}\setminus\{i,j\}}(\lambda_j-\lambda_k)} - \frac{f(\lambda_i)}{\prod_{k\in\{1,\dots,p\}\setminus\{i,j\}}(\lambda_i-\lambda_k)}\Bigg).$$

Proof. Without loss of generality, we may assume that $\lambda_i = \lambda_p$. By Proposition 2.2(2),

$$\Delta^{(p-1)}_{\lambda_1,\dots,\lambda_{p-1},s}(f) = \sum_{j=1}^{p-1} \frac{f(\lambda_j)}{\prod_{k\in\{1,\dots,p-1\}\setminus\{j\}}(\lambda_j-\lambda_k)(\lambda_j-s)} + \frac{f(s)}{\prod_{k\in\{1,\dots,p-1\}}(s-\lambda_k)}.$$

Next,

$$\begin{aligned}\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p-1},\lambda_p,\lambda_p}(f) &= \frac{\partial}{\partial s}\big(\Delta^{(p-1)}_{\lambda_1,\dots,\lambda_{p-1},s}(f)\big)\Big|_{s=\lambda_p} \\ &= \sum_{j=1}^{p-1} \frac{f(\lambda_j)}{\prod_{k\in\{1,\dots,p-1\}\setminus\{j\}}(\lambda_j-\lambda_k)(\lambda_p-\lambda_j)^2} \\ &\quad + \frac{f'(\lambda_p)}{\prod_{k\in\{1,\dots,p-1\}}(\lambda_p-\lambda_k)} \\ &\quad - f(\lambda_p)\sum_{j=1}^{p-1} \frac{1}{\prod_{k\in\{1,\dots,p-1\}\setminus\{j\}}(\lambda_p-\lambda_k)(\lambda_p-\lambda_j)^2},\end{aligned}$$

which coincides (upon regrouping the terms) with the expression in the statement of the lemma. □

In the case of repeated knots, the order of the divided difference can be reduced, as it is done in the next lemma.

LEMMA 2.4. *Let $f \in C^p[a,b]$ and $\lambda_1, \dots, \lambda_p \in [a,b]$. Then,*

$$\sum_{i=1}^{p} \Delta^{(p)}_{\lambda_1,\dots,\lambda_p,\lambda_i}(f) = \Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}(f').$$

Proof. In view of Proposition 2.2(4), it is enough to prove the lemma only in the case when all $\lambda_1,\dots,\lambda_p$ are distinct. Applying Lemma 2.3(4) ensures

$$\begin{aligned}(2.1)\qquad &\sum_{i=1}^{p}\Delta^{(p)}_{\lambda_1,\dots,\lambda_p,\lambda_i}(f)\\ &\quad=\sum_{i=1}^{p}\frac{f'(\lambda_i)}{\prod_{k\in\{1,\dots,p\}\setminus\{i\}}(\lambda_i-\lambda_k)}\\ &\qquad+\sum_{i=1}^{p}\sum_{j\in\{1,\dots,p\}\setminus\{i\}}\frac{1}{(\lambda_i-\lambda_j)^2}\Bigg(\frac{f(\lambda_j)}{\prod_{k\in\{1,\dots,p\}\setminus\{i,j\}}(\lambda_j-\lambda_k)}\\ &\qquad-\frac{f(\lambda_i)}{\prod_{k\in\{1,\dots,p\}\setminus\{i,j\}}(\lambda_i-\lambda_k)}\Bigg).\end{aligned}$$

By Proposition 2.2(2), the first summand in (2.1) equals $\Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}(f')$. The second summand in (2.1) with double summation sign equals zero; to see it, we group and cancel the terms with indices $(i,j)=(i_1,i_2)$ and $(i,j)=(i_2,i_1)$, where $i_1\neq i_2\in\{1,\dots,p\}$. ☐

Remark 2.5. Depending on the number of repeated knots of the divided difference in Proposition 2.2(4) and, subsequently, in Lemma 2.4, the smoothness assumption on f can be relaxed; see for details [5, Theorem 6.2 and Theorem 6.3].

The divided difference of a function in $\mathcal{W}_p(\mathbb{R})$ admits a useful representation as an integral of products of exponentials, each depending on only one knot of the divided difference.

Proposition 2.6 (See [1, Lemma 2.3]). *For $f\in\mathcal{W}_p(\mathbb{R})$,*

$$\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}(f)=\int_{\Pi^{(p)}}e^{\mathrm{i}(s_0-s_1)\lambda_1}\cdots e^{\mathrm{i}(s_{p-1}-s_p)\lambda_p}e^{\mathrm{i}s_p\lambda_{p+1}}\,d\sigma_f^{(p)}(s_0,\dots,s_p).$$

Here

$$\begin{aligned}\Pi^{(p)}=\big\{&(s_0,s_1,\dots,s_p)\in\mathbb{R}^{p+1}:|s_p|\le\cdots\le|s_1|\le|s_0|,\\ &\operatorname{sign}(s_0)=\cdots=\operatorname{sign}(s_p)\big\}\end{aligned}$$

and

$$d\sigma_f^{(p)}(s_0,s_1,\dots,s_p)=\mathrm{i}^p\mu_f(ds_0)\,ds_1\cdots ds_p,$$

where $f(t)=\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}e^{\mathrm{i}t\lambda}\,d\mu_f(\lambda)$.

Below, we list properties of piecewise polynomials, which will appear in representations for the higher order spectral shift functions, and include a representation of the divided difference in terms of its Peano kernel.

PROPOSITION 2.7.

(1) (*See* [5, Section 5.2(2.3) and (2.6)].) *The basic spline with the break points* $\lambda_1,\dots,\lambda_{p+1}$, *where at least two of the values are distinct, is defined by*

$$t \mapsto \begin{cases} \frac{1}{|\lambda_2-\lambda_1|}\chi_{(\min\{\lambda_1,\lambda_2\},\max\{\lambda_1,\lambda_2\})}(t) & \text{if } p=1,\\ \Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}\big((\lambda-t)_+^{p-1}\big) & \text{if } p>1.\end{cases}$$

Here the truncated power is defined by

$$x_+^k = \begin{cases} x^k & \text{if } x\ge 0,\\ 0 & \text{if } x<0,\end{cases} \quad \text{for } k\in\mathbb{N}.$$

The basic spline is nonnegative, supported in

$$\big[\min\{\lambda_1,\dots,\lambda_{p+1}\},\max\{\lambda_1,\dots,\lambda_{p+1}\}\big]$$

and integrable with the integral equal to $1/p$. (*Often the basic spline is normalized so that its integral equals* 1.)

(2) (*See* [5, Section 5.2, (2.2) and Section 4.7(c)].) *Let* $[a,b]\supseteq[\min\{\lambda_1,\dots,\lambda_{p+1}\},\max\{\lambda_1,\dots,\lambda_{p+1}\}]$. *For* $f\in C^p[a,b]$,

$$\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}(f) = \begin{cases} \frac{1}{(p-1)!}\int_a^b f^{(p)}(t)\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}\big((\lambda-t)_+^{p-1}\big)\,dt \\ \quad \text{if } \exists i_1,i_2 \text{ such that } \lambda_{i_1}\neq\lambda_{i_2},\\ \frac{1}{p!}f^{(p)}(\lambda_1)\\ \quad \text{if } \lambda_1=\lambda_2=\dots=\lambda_{p+1}.\end{cases} \tag{2.2}$$

The first equality in (2.2) *also holds for* $f\in C^{p-1}[a,b]$, *with* $f^{(p-1)}$ *absolutely continuous and* $f^{(p)}$ *integrable on* $[a,b]$.

Properties of an antiderivative of the basic spline are written below.

PROPOSITION 2.8 (See [16, Lemma 3.1]).

(i) *If* $\lambda_1=\dots=\lambda_{p+1}\in\mathbb{R}$, *with* $p\ge 0$, *then*

$$\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}\big((\lambda-t)_+^{p}\big)=\chi_{(-\infty,\lambda_1)}(t). \tag{2.3}$$

(ii) *If not all* $\lambda_1,\dots,\lambda_{p+1}\in\mathbb{R}$ *coincide, let* $\mathcal{I}$ *be the set of indices* i *for which* λ_i *are distinct and let* $m(\lambda_i)$ *be the multiplicity of* λ_i. *Assume that* $p\ge 1$ *and* $M=\max_{i\in\mathcal{I}} m(\lambda_i)\le p$. *Then,* $t\mapsto\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}((\lambda-t)_+^p)\in C^{p-M}(\mathbb{R})$ *and*

$$\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}\big((\lambda-t)_+^{p}\big)=p\int_t^\infty \Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}\big((\lambda-s)_+^{p-1}\big)\,ds. \tag{2.4}$$

PROPOSITION 2.9 (See [16, Lemma 3.2]). *Let* $(\lambda_1,\dots,\lambda_{p+1})\in\mathbb{R}^{p+1}$. *Then the function* $\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}((\lambda-t)_+^p)$ *is decreasing; it is equal to* 1 *when* $t<\min_{1\le k\le p+1}\lambda_k$ *and equal to* 0 *when* $t\ge\max_{1\le k\le p+1}\lambda_k$.

We will need a representation of the divided difference in terms of an antiderivative of the corresponding basic spline (2.4).

LEMMA 2.10. *Let* $[a,b] \supseteq [\min\{\lambda_1,\ldots,\lambda_{p+1}\},\max\{\lambda_1,\ldots,\lambda_{p+1}\}]$. *For* $f \in C^{p+1}[a,b]$,

$$\Delta^{(p)}_{\lambda_1,\ldots,\lambda_{p+1}}(f) = \frac{1}{p!}f^{(p)}(a) + \frac{1}{p!}\int_a^b f^{(p+1)}(t)\Delta^{(p)}_{\lambda_1,\ldots,\lambda_{p+1}}\big((\lambda-t)_+^p\big)\,dt. \tag{2.5}$$

Proof. Assume first that not all $\lambda_1,\ldots,\lambda_{p+1}$ coincide. Applying Proposition 2.7(2) and then integrating by parts and applying the representation (2.4) of Proposition 2.8 provide

$$\begin{aligned}
&\Delta^{(p)}_{\lambda_1,\ldots,\lambda_{p+1}}(f)\\
&\quad= \frac{1}{(p-1)!}\int_a^b f^{(p)}(t)\Delta^{(p)}_{\lambda_1,\ldots,\lambda_{p+1}}\big((\lambda-t)_+^{p-1}\big)\,dt\\
&\quad= -\frac{1}{p!}\big(f^{(p)}(t)\Delta^{(p)}_{\lambda_1,\ldots,\lambda_{p+1}}\big((\lambda-t)_+^p\big)\big)\Big|_a^b\\
&\qquad+ \frac{1}{p!}\int_a^b f^{(p+1)}(t)\Delta^{(p)}_{\lambda_1,\ldots,\lambda_{p+1}}\big((\lambda-t)_+^p\big)\,dt.
\end{aligned}$$

By Proposition 2.9, the latter reduces to (2.5). If $\lambda_1 = \cdots = \lambda_{p+1}$, then by Proposition 2.7(2),

$$\Delta^{(p)}_{\lambda_1,\ldots,\lambda_1}(f) = \frac{1}{p!}f^{(p)}(\lambda_1) = \frac{1}{p!}f^{(p)}(a) + \frac{1}{p!}\int_a^{\lambda_1} f^{(p+1)}(t)\,dt.$$

With use of the representation (2.3) of Proposition 2.8, the latter can be rewritten as (2.5). □

3. Traces of multiple operator integrals

In this section, we represent traces of certain multiple operator integrals as multiple scalar integrals. In particular, we obtain useful formulas for the traces of the Gâteaux derivatives $\tau[\frac{d^p}{dx^p}f(H_0+xV)]$, where $V=V^*$ is a Hilbert–Schmidt perturbation of a self-adjoint operator H_0 and $f \in \mathcal{W}_p(\mathbb{R})$.

3.1. Multiple spectral measures. We will need the facts that certain multi-measures extend to finite countably additive measures.

PROPOSITION 3.1. *Let* $2 \le p \in \mathbb{N}$ *and let* $E_1, E_2, \ldots, E_p$ *be projection-valued Borel measures from* $\mathbb{R}$ *to* $\mathcal{M}$. *Suppose that* $V_1,\ldots,V_p$ *belong to* $\mathcal{L}_2(\mathcal{M},\tau)$. *Assume that either* $\mathcal{M}=\mathcal{B}(\mathcal{H})$ *or* $p=2$. *Then there is a unique (complex) Borel measure* m *on* $\mathbb{R}^p$ *with total variation not exceeding the product* $\|V_1\|_2\|V_2\|_2\cdots\|V_p\|_2$, *whose value on rectangles is given by*

$$m(A_1\times A_2\times\cdots\times A_p) = \tau\big[E_1(A_1)V_1E_2(A_2)V_2\cdots V_{p-1}E_p(A_p)V_p\big]$$

for all Borel subsets $A_1, A_2, \ldots, A_p$ *of* $\mathbb{R}$.

Remark 3.2. In the case of $\mathcal{M} = \mathcal{B}(\mathcal{H})$ and V a Hilbert–Schmidt operator, Proposition 3.1 was obtained in [3], [11]. For a general $\mathcal{M}$ and $V \in \mathcal{L}_2(\mathcal{M}, \tau)$, the set function m is known to be of bounded variation only if $p = 2$ (see [6, Section 4] for a positive result and a counterexample).

Proposition 3.3 (See [6, Corollary 4.3]). *Under the assumptions of Proposition 3.1, there is a unique (complex) Borel measure m_1 on $\mathbb{R}^p$ with total variation not exceeding the product $\|V_1\|_2\|V_2\|_2 \cdots \|V_p\|_2$, whose value on rectangles is given by*

$$\begin{aligned} &m_1(A_1 \times A_2 \times \cdots \times A_p \times A_{p+1}) \\ &\quad = \tau\big[E_1(A_1)V_1E_2(A_2)V_2 \cdots V_{p-1}E_p(A_p)V_pE_1(A_{p+1})\big] \end{aligned}$$

for all Borel subsets $A_1, A_2, \dots, A_p, A_{p+1}$ of $\mathbb{R}$.

In the sequel, we will work with the set functions

$$\begin{aligned} &m_{p,H_0,V}(A_1 \times A_2 \times \cdots \times A_p) = \tau\big[E_{H_0}(A_1)VE_{H_0}(A_2)V \cdots VE_{H_0}(A_p)V\big], \\ &m^{(1)}_{p,H_0,V}(A_1 \times A_2 \times \cdots \times A_{p+1}) \\ &\quad = \tau\big[E_{H_0}(A_1)VE_{H_0}(A_2)V \cdots VE_{H_0}(A_p)VE_{H_0}(A_{p+1})\big] \end{aligned}$$

and their countably-additive extensions (when they exist), called multiple spectral measures. Here A_j, $1 \le j \le p$, are measurable subsets of $\mathbb{R}$, $H_0 = H_0^*$ is affiliated with $\mathcal{M}$, E_{H_0} is the spectral measure of H_0, and $V = V^* \in \mathcal{L}_2(\mathcal{M}, \tau)$. Clearly, the measures $m_{p,H_0,V}$ and $m^{(1)}_{p,H_0,V}$ are particular representatives of the measures m and m_1, respectively.

Proposition 3.4 (See [6, Theorem 4.5]). *Let τ be a finite trace normalized by $\tau(I) = 1$ and let $H_0 = H_0^*$ be affiliated with $\mathcal{M}$ and $V = V^* \in \mathcal{M}$. Assume that $(zI - H_0)^{-1}$ and V are free. Then the set functions $m_{p,H_0,V}$ and $m^{(1)}_{p,H_0,V}$ extend to countably additive measures of bounded variation.*

Upon evaluating a trace, some iterated operator integrals can be written as Lebesgue integrals with respect to "multiple spectral measures".

Proposition 3.5 (See [6, Lemma 4.9]). *Assume the hypothesis of Proposition 3.1. Assume that the spectral measures $E_1, E_2, \dots, E_p$ correspond to self-adjoint operators $H_0, H_1, \dots, H_p$ affiliated with $\mathcal{M}$, respectively, and that $V_1, V_2, \dots, V_p \in \mathcal{L}_2(\mathcal{M}, \tau)$. Let $f_1, f_2, \dots, f_p$ be functions in $C_b(\mathbb{R})$ (continuous bounded). Then*

$$\begin{aligned} &\tau\big[f_1(H_1)V_1f_2(H_2)V_2 \cdots f_p(H_p)V_p\big] \\ &\quad = \int_{\mathbb{R}^p} f_1(\lambda_1)f_2(\lambda_2) \cdots f_p(\lambda_p)\, dm(\lambda_1, \lambda_2, \dots, \lambda_p), \end{aligned}$$

with m as in Proposition 3.1.

Remark 3.6. A completely analogous result with m replaced by m_1, $m_{p,H_0,V}$ or $m^{(1)}_{p,H_0,V}$ holds under the hypothesis of Proposition 3.1 or Proposition 3.4.

3.2. Reduction of traces of multiple operator integrals to scalar integrals.

DEFINITION 3.7 ([1, Definition 4.1]; see also [14]). Let $H_k = H_k^*$ and $V_k = V_k^*$, with $k = 1, \dots, p+1$, be operators defined in $\mathcal{H}$. Assume that V_k, $k = 1, \dots, p+1$, are bounded. Let ϕ be a function representable in the form

$$\begin{aligned}(3.1)\qquad &\phi(\lambda_1, \lambda_2, \dots, \lambda_p, \lambda_{p+1})\\ &= \int_S \alpha_1(\lambda_1, s)\alpha_2(\lambda_2, s)\cdots\alpha_p(\lambda_p, s)\alpha_{p+1}(\lambda_{p+1}, s)\, d\sigma(s),\end{aligned}$$

where (S, σ) is a finite measure space and $\alpha_1, \dots, \alpha_{p+1}$ are bounded Borel functions on $\mathbb{R} \times S$. Then the multiple operator integral

$$\begin{aligned}\int_{\mathbb{R}^{p+1}} &\phi(\lambda_1, \lambda_2, \dots, \lambda_p, \lambda_{p+1})\, dE_{H_1}(\lambda_1)V_1\, dE_{H_2}(\lambda_2)V_2 \cdots\\ &dE_{H_p}(\lambda_p)V_p\, dE_{H_{p+1}}(\lambda_{p+1})\end{aligned}$$

is defined as the Bochner integral

$$\int_S \alpha_1(H_1, s)V_1\alpha_2(H_2, s)V_2 \cdots \alpha_p(H_p, s)V_p\alpha_{p+1}(H_{p+1}, s)\, d\sigma(s).$$

When the set functions m and m_1 admit extensions to finite countably additive measures, a trace of a multiple operator integral can be represented as a multiple scalar integral.

LEMMA 3.8. *Let $H_1, \dots, H_{p+1}$ be self-adjoint operators affiliated with $\mathcal{M}$ and $V_1, \dots, V_p$ self-adjoint operators in $\mathcal{L}_2(\mathcal{M}, \tau)$. Let $E_k = E_{H_k}$, for $k = 1, \dots, p+1$, and let ϕ be a bounded Borel function admitting the representation* (3.1). *Then, the following representations hold.*

(1) *For m_1 the measure provided by Proposition 3.3 or Proposition 3.4,*

$$\begin{aligned}\tau\Big[\int_{\mathbb{R}^{p+1}} &\phi(\lambda_1, \dots, \lambda_p, \lambda_{p+1})\, dE_{H_1}(\lambda_1)V_1 \cdots dE_{H_p}(\lambda_p)V_p\, dE_{H_{p+1}}(\lambda_{p+1})\Big]\\ &= \int_{\mathbb{R}^{p+1}} \phi(\lambda_1, \dots, \lambda_p, \lambda_{p+1})\, dm_1(\lambda_1, \dots, \lambda_p, \lambda_{p+1}).\end{aligned}$$

(2) *In the case $H_{p+1} = H_1$, for m the measure provided by Proposition 3.1 or Proposition 3.4,*

$$\begin{aligned}\tau\Big[\int_{\mathbb{R}^{p+1}} &\phi(\lambda_1, \lambda_2, \dots, \lambda_p, \lambda_{p+1})\, dE_{H_1}(\lambda_1)V_1\, dE_{H_2}(\lambda_2)V_2 \cdots\\ &dE_{H_p}(\lambda_p)V_p\, dE_{H_1}(\lambda_{p+1})\Big]\\ &= \int_{\mathbb{R}^p} \phi(\lambda_1, \lambda_2, \dots, \lambda_p, \lambda_1)\, dm(\lambda_1, \lambda_2, \dots, \lambda_p).\end{aligned}$$

(3) *For m the measure provided by Proposition 3.1 or Proposition 3.4,*

$$\tau\left[V_{p+1}\int_{\mathbb{R}^{p+1}}\phi(\lambda_1,\dots,\lambda_p,\lambda_{p+1})\,dE_{H_1}(\lambda_1)V_1\cdots dE_{H_p}(\lambda_p)V_p\,dE_{H_{p+1}}(\lambda_{p+1})\right]$$
$$=\int_{\mathbb{R}^p}\phi(\lambda_1,\dots,\lambda_p,\lambda_{p+1})\,dm(\lambda_1,\dots,\lambda_p,\lambda_{p+1}).$$

Proof. (1) By [1, Lemma 3.10 and Remark 4.2],

$$\tau\left[\int_S\alpha_1(H_1,s)V_1\cdots\alpha_p(H_p,s)V_p\alpha_{p+1}(H_{p+1},s)\,d\sigma(s)\right]$$
$$=\int_S\tau\big[\alpha_1(H_1,s)V_1\cdots\alpha_p(H_p,s)V_p\alpha_{p+1}(H_{p+1},s)\big]\,d\sigma(s).$$

By Remark 3.6, the latter integral equals

$$\int_S\int_{\mathbb{R}^{p+1}}\alpha_1(\lambda_1,s)\cdots\alpha_p(\lambda_p,s)\alpha_{p+1}(\lambda_{p+1},s)\,dm_1(\lambda_1,\dots,\lambda_p,\lambda_{p+1})\,d\sigma(s),$$

which by Fubini's theorem converts to

$$\int_{\mathbb{R}^{p+1}}\int_S\alpha_1(\lambda_1,s)\cdots\alpha_p(\lambda_p,s)\alpha_{p+1}(\lambda_{p+1},s)\,d\sigma(s)\,dm_1(\lambda_1,\dots,\lambda_p,\lambda_{p+1})$$
$$=\int_{\mathbb{R}^{p+1}}\phi(\lambda_1,\dots,\lambda_p,\lambda_{p+1})\,dm_1(\lambda_1,\dots,\lambda_p,\lambda_{p+1}).$$

(2) By [1, Lemma 3.10 and Remark 4.2] and cyclicity of the trace,

$$\tau\left[\int_S\alpha_1(H_1,s)V_1\alpha_2(H_2,s)\cdots V_p\alpha_{p+1}(H_{p+1},s)\,d\sigma(s)\right]$$
$$=\int_S\tau\big[\alpha_{p+1}(H_1,s)\alpha_1(H_1,s)V_1\alpha_2(H_2,s)\cdots V_p\big]\,d\sigma(s).$$

By Proposition 3.5, the latter integral equals

$$\int_S\int_{\mathbb{R}^p}\alpha_{p+1}(\lambda_1,s)\alpha_1(\lambda_1,s)\alpha_2(\lambda_2,s)\cdots\alpha_p(\lambda_p,s)\,dm(\lambda_1,\lambda_2,\dots,\lambda_p)\,d\sigma(s),$$

which by Fubini's theorem converts to

$$\int_{\mathbb{R}^p}\int_S\alpha_1(\lambda_1,s)\alpha_2(\lambda_2,s)\cdots\alpha_p(\lambda_p,s)\alpha_{p+1}(\lambda_1,s)\,d\sigma(s)\,dm(\lambda_1,\lambda_2,\dots,\lambda_p)$$
$$=\int_{\mathbb{R}^p}\phi(\lambda_1,\lambda_2,\dots,\lambda_p,\lambda_1)\,dm(\lambda_1,\lambda_2,\dots,\lambda_p).$$

(3) By [1, Lemma 3.7]

$$\tau\left[V_{p+1}\int_{\mathbb{R}^{p+1}}\phi(\lambda_1,\dots,\lambda_p,\lambda_{p+1})\,dE_{H_1}(\lambda_1)V_1\cdots dE_{H_p}(\lambda_p)V_p\,dE_{H_{p+1}}(\lambda_{p+1})\right]$$
$$=\tau\left[\int_S V_{p+1}\alpha_1(H_1,s)V_1\cdots\alpha_p(H_p,s)V_p\alpha_{p+1}(H_{p+1},s)\,d\sigma(s)\right].$$

By following the lines of the proof of (1), we obtain that the latter equals

$$\begin{aligned}&\int_S \tau\left[V_{p+1}\alpha_1(H_1,s)V_1\cdots\alpha_p(H_p,s)V_p\alpha_{p+1}(H_{p+1},s)\right]d\sigma(s)\\&\quad=\int_{\mathbb{R}^p}\phi(\lambda_1,\dots,\lambda_p,\lambda_{p+1})\,dm(\lambda_1,\dots,\lambda_p,\lambda_{p+1}).\end{aligned}$$

□

REMARK 3.9. If in the statement of Lemma 3.8(2), we change the assumption $V_1,\dots,V_p\in\mathcal{L}_2(\mathcal{M},\tau)$ to $V_1,\dots,V_p\in\mathcal{L}_p(\mathcal{M},\tau)$, then we obtain

$$\begin{aligned}&\tau\Bigg[\int_{\mathbb{R}^{p+1}}\phi(\lambda_1,\lambda_2,\dots,\lambda_p,\lambda_{p+1})\,dE_{H_1}(\lambda_1)V_1\,dE_{H_2}(\lambda_2)V_2\cdots\\&\qquad dE_{H_p}(\lambda_p)V_p\,dE_{H_1}(\lambda_{p+1})\Bigg]\\&\quad=\tau\left[\int_{\mathbb{R}^p}\phi(\lambda_1,\lambda_2,\dots,\lambda_p,\lambda_1)\,dE_{H_1}(\lambda_1)V_1\,dE_{H_2}(\lambda_2)V_2\cdots dE_{H_p}(\lambda_p)V_p\right].\end{aligned}$$

We have the following representation for the derivative $\frac{d^p}{dx^p}f(H_0+xV)$.

PROPOSITION 3.10 ([14, Theorem 5.6]; see also [1, Theorem 5.7]). *Let $H_0=H_0^*$ be an operator affiliated with $\mathcal{M}$ and $V=V^*$ an operator in $\mathcal{M}$. Then for every f in $\mathcal{W}_p(\mathbb{R})$,*

$$\frac{d^p}{dx^p}\bigg|_{x=0}f(H_0+xV)=p!\int_{\mathbb{R}^{p+1}}\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}(f)\,dE_{H_0}(\lambda_1)V\cdots V\,dE_{H_0}(\lambda_{p+1}).$$

The main assumptions of the following results are collected in the format of a hypothesis.

HYPOTHESIS 3.11. *Let $H_0=H_0^*$ be affiliated with $\mathcal{M}$ and $V=V^*\in\mathcal{L}_2(\mathcal{M},\tau)$. Assume that one of the following three conditions is satisfied*:

(1) $\mathcal{M}=\mathcal{B}(\mathcal{H})$, $p\geq 2$,
(2) $2\leq p\leq 3$,
(3) *$\mathcal{M}$ is finite, $p\geq 2$, and $(zI-H_0)^{-1}$ and V are free in $(\mathcal{M},\tau)$.*

In the multiple operator integral representation for the derivative $\frac{d^p}{dx^p}f(H_0+xV)$ provided by Proposition 3.10, the order of the divided difference can be reduced upon evaluating the trace.

THEOREM 3.12. *Assume Hypothesis 3.11. Then for $f\in\mathcal{W}_p(\mathbb{R})$,*

$$\begin{aligned}&\tau\left[\frac{d^p}{dx^p}\bigg|_{x=0}f(H_0+xV)\right]\\&\quad=p!\int_{\mathbb{R}^{p+1}}\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}(f)\,dm^{(1)}_{p,H_0,V}(\lambda_1,\dots,\lambda_{p+1})\end{aligned}\tag{3.2}$$

$$\quad=(p-1)!\int_{\mathbb{R}^p}\Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}\left(f'\right)dm_{p,H_0,V}(\lambda_1,\dots,\lambda_p).\tag{3.3}$$

Proof. By Proposition 2.6, the function $\phi(\lambda_1,\dots,\lambda_{p+1}) = \Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}(f)$ admits the representation (3.1), where $\alpha_1(\lambda_1,s) = e^{\mathrm{i}(s_0-s_1)\lambda_1},\dots,\alpha_p(\lambda_p,s) = e^{\mathrm{i}(s_{p-1}-s_p)\lambda_p}$, and $\alpha_{p+1}(\lambda_{p+1},s) = e^{\mathrm{i}s_p\lambda_{p+1}}$. It follows from Proposition 3.10 and Lemma 3.8 that

$$\tau\left[\frac{d^p}{dx^p}\bigg|_{x=0} f(H_0+xV)\right]$$

$$= \tau\left[\int_{\mathbb{R}^{p+1}} \Delta^{(p)}_{\lambda_1,\lambda_2,\dots,\lambda_p,\lambda_{p+1}}(f)\, dE_{H_0}(\lambda_1)V\, dE_{H_0}(\lambda_2)V\cdots V\, dE_{H_0}(\lambda_{p+1})\right]$$

$$= \int_{\mathbb{R}^{p+1}} \Delta^{(p)}_{\lambda_1,\lambda_2,\dots,\lambda_p,\lambda_{p+1}}(f)\, dm^{(1)}_{p,H_0,V}(\lambda_1,\lambda_2,\dots,\lambda_p,\lambda_{p+1}) \tag{3.4}$$

$$= \int_{\mathbb{R}^{p}} \Delta^{(p)}_{\lambda_1,\lambda_2,\dots,\lambda_p,\lambda_1}(f)\, dm_{p,H_0,V}(\lambda_1,\lambda_2,\dots,\lambda_p). \tag{3.5}$$

Proposition 3.10 and the representation (3.4) imply (3.2).

To prove that the expressions in (3.2) and (3.3) are equal, we note first that a trivial renumbering of the variables of integration gives

$$\begin{aligned}\int_{\mathbb{R}^{p}} &\Delta^{(p)}_{\lambda_1,\lambda_2,\dots,\lambda_p,\lambda_1}(f)\, dm_{p,H_0,V}(\lambda_1,\lambda_2,\dots,\lambda_p)\\ &= \int_{\mathbb{R}^{p}} \Delta^{(p)}_{\lambda_i,\lambda_{i+1},\dots,\lambda_p,\lambda_1,\dots,\lambda_{i-1},\lambda_i}(f)\, dm_{p,H_0,V}(\lambda_i,\lambda_{i+1},\dots,\\ &\qquad \lambda_p,\lambda_1,\dots,\lambda_{i-1}).\end{aligned} \tag{3.6}$$

Cyclicity of the trace τ ensures cyclicity of the measure $m_{p,H_0,V}$, that is,

$$\begin{aligned}&dm_{p,H_0,V}(\lambda_i,\lambda_{i+1},\dots,\lambda_p,\lambda_1,\dots,\lambda_{i-1})\\ &\qquad = dm_{p,H_0,V}(\lambda_1,\dots,\lambda_{i-1},\lambda_i,\lambda_{i+1},\dots,\lambda_p).\end{aligned} \tag{3.7}$$

Symmetry of the divided difference (see Proposition 2.2(1)) along with (3.6) and (3.7) ensures the equality

$$\begin{aligned}\int_{\mathbb{R}^{p}} &\Delta^{(p)}_{\lambda_1,\lambda_2,\dots,\lambda_p,\lambda_1}(f)\, dm_{p,H_0,V}(\lambda_1,\lambda_2,\dots,\lambda_p)\\ &= \int_{\mathbb{R}^{p}} \Delta^{(p)}_{\lambda_1,\lambda_2,\dots,\lambda_p,\lambda_i}(f)\, dm_{p,H_0,V}(\lambda_1,\lambda_2,\dots,\lambda_p).\end{aligned} \tag{3.8}$$

It follows from (3.8) and Lemma 2.4 that

$$\begin{aligned}p\int_{\mathbb{R}^{p}} &\Delta^{(p)}_{\lambda_1,\lambda_2,\dots,\lambda_p,\lambda_1}(f)\, dm_{p,H_0,V}(\lambda_1,\lambda_2,\dots,\lambda_p)\\ &= \sum_{i=1}^{p}\int_{\mathbb{R}^{p}} \Delta^{(p)}_{\lambda_1,\lambda_2,\dots,\lambda_p,\lambda_i}(f)\, dm_{p,H_0,V}(\lambda_1,\lambda_2,\dots,\lambda_p)\\ &= \int_{\mathbb{R}^{p}} \Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}(f')\, dm_{p,H_0,V}(\lambda_1,\dots,\lambda_p).\end{aligned} \tag{3.9}$$

Combination of (3.5) and (3.9) completes the proof of the theorem. □

As an application of Theorem 3.12, we obtain positivity of Koplienko's spectral shift function in the von Neumann algebra setting. In the $\mathcal{B}(\mathcal{H})$ setting, positivity of $\eta = \eta_2$ was obtained in [7] and in the extended setting for $V \in \mathcal{L}_1(\mathcal{M}, \tau)$ in [15].

COROLLARY 3.13. *Let $H_0 = H_0^*$ be affiliated with $\mathcal{M}$ and $V = V^* \in \mathcal{L}_2(\mathcal{M}, \tau)$. Then $\eta_2 \geq 0$.*

Proof. Due to Koplienko's trace formula (1.2), it is enough to show that

$$\tau\left[f(H_1) - f(H_0) - \frac{d}{dx}\bigg|_{x=0} f(H_0 + xV)\right] \geq 0$$

for every $f \in C_c^3(\mathbb{R}) \subset \mathcal{W}_2(\mathbb{R})$, with $f'' \geq 0$. We have the integral representation

$$\begin{aligned} \tau\left[f(H_1) - f(H_0) - \frac{d}{dx}\bigg|_{x=0} f(H_0 + xV)\right] \\ = \int_0^1 (1-x)\tau\left[\frac{d^2}{dx^2} f(H_0 + xV)\right] dx \end{aligned} \tag{3.10}$$

(see, e.g., [6, Theorem 11 and Lemma 3.11]). Further, by (3.3) of Theorem 3.12 with $p = 2$, for every $f \in \mathcal{W}_2(\mathbb{R})$,

$$\tau\left[\frac{d^2}{dx^2} f(H_0 + xV)\right] = \int_{\mathbb{R}^2} \Delta^{(1)}_{\lambda_0,\lambda_1}\big(f'\big)\, dm_{2,H_0+xV,V}(\lambda_0, \lambda_1). \tag{3.11}$$

It is easy to derive that the measure $m_{2,H_0+xV,V}$ is nonnegative, for every $x \in [0,1]$ (see, e.g., [6, Lemma 4.7]). If $f'' \geq 0$, then f' is increasing and $\Delta^{(1)}_{\lambda_0,\lambda_1}(f') \geq 0$ for all λ_0, λ_1. (The latter follows, for instance, from Proposition 2.7.) Thus, if $f'' \geq 0$, then the expressions in (3.11) and (3.10) are nonnegative, which completes the proof. □

COROLLARY 3.14. *Assume Hypothesis 3.11. Assume, in addition, that H_0 is bounded. Let $[a,b]$ be a segment containing $\sigma(H_0) \cup \sigma(H_0 + V)$. Then for $f \in \mathcal{W}_p(\mathbb{R}) \cap C^{p+1}(\mathbb{R})$,*

$$\tau\left[\frac{d^p}{dx^p}\bigg|_{x=0} f(H_0 + xV)\right] - \tau\big(V^p\big) f^{(p)}(a)$$

$$= \int_a^b f^{(p+1)}(t) \int_{[a,b]^{p+1}} \Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}\big((\lambda - t)_+^p\big)\, dm^{(1)}_{p,H_0,V}(\lambda_1, \dots, \lambda_{p+1})\, dt \tag{3.12}$$

$$= \int_a^b f^{(p+1)}(t) \int_{[a,b]^p} \Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}\big((\lambda - t)_+^{p-1}\big)\, dm_{p,H_0,V}(\lambda_1, \dots, \lambda_p)\, dt. \tag{3.13}$$

Proof. First, note that the measure $m_{p,H_0,V}$ is supported in $[a,b]^p$. Expanding the integrands in (3.2) and (3.3) according to (2.5) of Lemma 2.10 and then using Fubini's theorem (the functions $f^{(p+1)}(\cdot)$, $\Delta^{(p)}_{\lambda_1,\dots,\lambda_{p+1}}((\lambda-\cdot)^p_+)$, and $\Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}((\lambda-\cdot)^{p-1}_+)$ are bounded and the measures $m^{(1)}_{p,H_0,V}$ and $m_{p,H_0,V}$ are finite) provide the representations (3.12) and (3.13). Here we used the fact that $m^{(1)}_{p,H_0,V}(\mathbb{R}^{p+1}) = m_{p,H_0,V}(\mathbb{R}^p) = \tau(V^p)$. □

The order of an operator derivative inside a trace can be decreased by means of increasing the order of a scalar derivative.

COROLLARY 3.15. *Assume Hypothesis* 3.11. *Then for* $f \in \mathcal{W}_p(\mathbb{R})$,

$$\tau\left[\frac{d^p}{dx^p}\bigg|_{x=0} f(H_0+xV)\right] = \tau\left[V\frac{d^{p-1}}{dx^{p-1}}\bigg|_{x=0} f'(H_0+xV)\right].$$

Proof. By Lemma 3.8(3) and Proposition 3.10,

$$\begin{aligned}(p-1)!\int_{\mathbb{R}^p} &\Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}\big(f'\big)\,dm_{p,H_0,V}(\lambda_1,\dots,\lambda_p)\\ &= \tau\left[V\frac{d^{p-1}}{dx^{p-1}}\bigg|_{x=0} f'(H_0+xV)\right],\end{aligned}$$

which along with Theorem 3.12 completes the proof. □

REMARK 3.16. The assertions of Corollaries 3.14 and 3.15 remain true if $p=1$, provided $V \in \mathcal{L}_1(\mathcal{M},\tau)$.

4. Properties of the spectral shift measure

In this section, we prove existence of the higher order spectral shift functions and derive some of their properties by implementing a multiple operator integral approach.

THEOREM 4.1. *Assume Hypothesis* 3.11. *Assume*, *in addition*, *that* H_0 *is bounded.*

(1) *There exists a unique finite real-valued absolutely continuous measure* ν_p *such that the trace formula*

$$\tau\big[R_p(f)\big] = \int_{\mathbb{R}} f^{(p)}(t)\,d\nu_p(t) \tag{4.1}$$

holds for $f \in \mathcal{W}_p(\mathbb{R}) \cup \mathfrak{R}$, *where* $\mathfrak{R}$ *denotes the set of rational functions on* $\mathbb{R}$ *with nonreal poles.*

(2) *The density of* ν_p *is given by the formulas*

$$\begin{aligned}\eta_p(t) &= \frac{\tau(V^{p-1})}{(p-1)!} - \nu_{p-1}\big((-\infty,t)\big)\\ &\quad - \frac{1}{(p-1)!}\int_{\mathbb{R}^p} \Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}\big((\lambda-t)^{p-1}_+\big)\,dm^{(1)}_{p-1,H_0,V}(\lambda_1,\dots,\lambda_p)\end{aligned} \tag{4.2}$$

$$= \frac{\tau(V^{p-1})}{(p-1)!} - \nu_{p-1}\big((-\infty,t)\big)$$

$$- \frac{1}{(p-1)!}\int_{\mathbb{R}^{p-1}} \Delta^{(p-2)}_{\lambda_1,\dots,\lambda_{p-1}}\big((\lambda-t)_+^{p-2}\big)\,dm_{p-1,H_0,V}(\lambda_1,\dots,\lambda_{p-1}). \tag{4.3}$$

(3) *The measure* ν_p *is supported in the convex hull of the set* $\sigma(H_0)\cup\sigma(H_0+V)$ *and* $\nu_p(\mathbb{R}) = \frac{\tau(V^p)}{p!}$.

REMARK 4.2. Theorem 4.1, except for the representation (4.2), was originally proved in [6, Theorem 5.1, Theorem 5.2, and Theorem 5.6]. We provide a shorter proof.

Proof of Theorem 4.1. The proof can be accomplished by induction. The result is known to hold for $p=2$ (see [6], [7]). Assume that the theorem holds when p is replaced with $p-1$. Let $[a,b]$ be a segment containing $\sigma(H_0)\cup\sigma(H_0+V)$. Then η_{p-1} is supported in $[a,b]$. Clearly,

$$\tau\big[R_p(f)\big] = \tau\big[R_{p-1}(f)\big] - \frac{1}{(p-1)!}\tau\left[\frac{d^{p-1}}{dx^{p-1}}\bigg|_{x=0} f(H_0+xV)\right]. \tag{4.4}$$

Let $f\in\mathcal{W}_p(\mathbb{R})$. By the induction hypothesis and the representation (3.12) of Corollary 3.14, the expression in (4.4) equals

$$\int_a^b f^{(p-1)}(t)\eta_{p-1}(t)\,dt - \frac{\tau(V^{p-1})}{(p-1)!}f^{(p-1)}(a) \tag{4.5}$$
$$- \frac{1}{(p-1)!}$$
$$\times \int_a^b f^{(p)}(t)\int_{[a,b]^p} \Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}\big((\lambda-t)_+^{p-1}\big)\,dm^{(1)}_{p-1,H_0,V}(\lambda_1,\dots,\lambda_p)\,dt.$$

Integrating by parts in the first integral in (4.5) gives

$$\int_{[a,b]} f^{(p-1)}(t)\eta_{p-1}(t)\,dt \tag{4.6}$$
$$= \left(f^{(p-1)}(t)\int_a^t \eta_{p-1}(s)\,ds\right)\bigg|_a^b - \int_a^b f^{(p)}(t)\left(\int_a^t \eta_{p-1}(s)\,ds\right)dt$$
$$= f^{(p-1)}(b)\frac{\tau(V^{p-1})}{(p-1)!} - \int_a^b f^{(p)}(t)\left(\int_a^t \eta_{p-1}(s)\,ds\right)dt.$$

Combining (4.4)–(4.6) implies

$$\tau\big[R_p(f)\big]$$
$$= \big(f^{(p-1)}(b) - f^{(p-1)}(a)\big)\frac{\tau(V^{p-1})}{(p-1)!} - \int_a^b f^{(p)}(t)\int_a^t \eta_{p-1}(s)\,ds\,dt$$
$$- \int_a^b f^{(p)}(t)\frac{1}{(p-1)!}$$

$$\times \int_{[a,b]^p} \Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}\big((\lambda-t)_+^{p-1}\big)\, dm^{(1)}_{p-1,H_0,V}(\lambda_1,\dots,\lambda_p)\, dt$$

$$= \int_a^b f^{(p)}(t)\bigg(\frac{\tau(V^{p-1})}{(p-1)!} - \nu_{p-1}\big((a,t)\big) - \frac{1}{(p-1)!}\int_{\mathbb{R}^p} \Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}\big((\lambda-t)_+^{p-1}\big)\, dm^{(1)}_{p-1,H_0,V}(\lambda_1,\dots,\lambda_p)\bigg)\, dt,$$

from what the trace formula (4.1) follows for $f \in \mathcal{W}_p(\mathbb{R})$, with

$$\eta_p(t) = \frac{\tau(V^{p-1})}{(p-1)!} - \nu_{p-1}\big((a,t)\big) - \frac{1}{(p-1)!}\int_{\mathbb{R}^p} \Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}\big((\lambda-t)_+^{p-1}\big)\, dm^{(1)}_{p-1,H_0,V}(\lambda_1,\dots,\lambda_p).$$

Let $[c,d]$ denote the convex hull of $\sigma(H_0)\cup\sigma(H_0+V)$. By the induction hypothesis, $\nu_{p-1}((-\infty,c)) = \nu_{p-1}((d,\infty)) = 0$ and $\nu_{p-1}([c,d]) = \frac{\tau(V^{p-1})}{(p-1)!}$. By Proposition 2.9,

$$\int_{\mathbb{R}^p} \Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}\big((\lambda-t)_+^{p-1}\big)\, dm^{(1)}_{p-1,H_0,V}(\lambda_1,\dots,\lambda_p) = \begin{cases} m^{(1)}_{p-1,H_0,V}\big(\mathbb{R}^p\big) = \frac{\tau(V^{p-1})}{(p-1)!} & \text{if } t<c,\\ 0 & \text{if } t>d.\end{cases}$$

Therefore, (4.2) holds and the measure ν_p is supported in $[c,d]$. To extend the trace formula (4.1) to f a polynomial, we apply (4.1) to a function $g \in \mathcal{W}_p(\mathbb{R})$, which coincides with f on a segment containing $\bigcup_{x\in[-1,1]}\sigma(H_0+xV)$, and get

$$\tau\big[R_p(f)\big] = \tau\big[R_p(g)\big] = \int_{\mathbb{R}} g^{(p)}\, d\nu_p(t) = \int_{\mathbb{R}} f^{(p)}(t)\, d\nu_p(t).$$

To obtain the equality $\nu_p(\mathbb{R}) = \frac{\tau(V^p)}{p!}$, we apply (4.1) to $f(t)=t^p$. The measure ν_p is finite since it is compactly supported and its density is bounded.

The proof of (4.3) is completely analogous to the proof of (4.2), where the only difference consists in applying (3.13) (instead of (3.12)) to the second summand in (4.4). □

The techniques used in the proof of Theorem 4.1 also work in the case of an unbounded operator H_0, provided $f^{(p)} \in L^1(\mathbb{R})$ and ν_{p-1} is known to be finite.

THEOREM 4.3. *Let $H_0 = H_0^*$ be an operator affiliated with $\mathcal{M}$, $V=V^*$ an operator in $\mathcal{L}_2(\mathcal{M},\tau)$ and $p=3$. Then for $f \in C_c^p(\mathbb{R})\cup\mathfrak{R}_b$, where $\mathfrak{R}_b$ is the subset of bounded functions in $\mathfrak{R}$, the representations (4.1)–(4.3) hold.*

Proof. The proof is very similar to the one of Theorem 4.1, so we provide only a brief sketch. Clearly,

$$\begin{aligned} (4.7)\qquad 0 &= \lim_{a\to-\infty,b\to\infty}\big(f^{(p-1)}(b)-f^{(p-1)}(a)\big)\frac{\tau(V^{p-1})}{(p-1)!} \\ &= \int_{\mathbb{R}} f^{(p)}(t)\frac{\tau(V^{p-1})}{(p-1)!}\,dt. \end{aligned}$$

By letting $a\to-\infty$ and $b\to\infty$ in (4.6), we obtain

$$(4.8)\qquad \int_{\mathbb{R}} f^{(p-1)}(t)\eta_{p-1}(t)\,dt = -\int_{\mathbb{R}} f^{(p)}(t)\left(\int_{-\infty}^{t}\eta_{p-1}(s)\,ds\right)dt.$$

By letting $a\to-\infty$ and $b\to\infty$ in (2.5), we obtain

$$\Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}(f) = \frac{1}{(p-1)!}\int_{\mathbb{R}} f^{(p)}(t)\Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}\big((\lambda-t)_+^{p-1}\big)\,dt$$

and, subsequently,

$$\begin{aligned} &\tau\left[\frac{d^{p-1}}{dx^{p-1}}\bigg|_{x=0} f(H_0+xV)\right] \\ (4.9)\qquad &= \int_{\mathbb{R}} f^{(p)}(t)\int_{\mathbb{R}^p}\Delta^{(p-1)}_{\lambda_1,\dots,\lambda_p}\big((\lambda-t)_+^{p-1}\big)\,dm^{(1)}_{p-1,H_0,V}(\lambda_1,\dots,\lambda_p)\,dt \\ (4.10)\qquad &= \int_{\mathbb{R}} f^{(p)}(t)\int_{\mathbb{R}^{p-1}}\Delta^{(p-2)}_{\lambda_1,\dots,\lambda_{p-1}}\big((\lambda-t)_+^{p-2}\big)\,dm_{p-1,H_0,V}(\lambda_1,\dots,\lambda_{p-1})\,dt \end{aligned}$$

(see the proof of Corollary 3.14).

We note that the integral $\int_{-\infty}^{t}\eta_{p-1}(s)\,ds$ is well defined since $\eta_{p-1}=\eta_2$ is integrable (see, e.g., discussion in the introductory section of [16]). Combining (4.7)–(4.10), as it was done in the case of a bounded H_0, completes the proof. □

Remark 4.4. The trace formula (4.1) for $f\in C_c^\infty(\mathbb{R})$ (in fact, $f\in C_c^{p+1}(\mathbb{R})$ also works) was obtained in [6, Theorem 5.2], without establishing the absolute continuity of the measure ν_3 when H_0 is unbounded. The trace formula

$$(4.11)\qquad \tau\big[R_3(f)\big] = \int_{\mathbb{R}} f'''(t)\eta_3(t)\,dt,$$

for an unbounded H_0, with η_3 given by (4.3), was proved in [16, Theorem 4.1] only for $f\in\mathfrak{R}_b$. The results of Theorem 3.12 have allowed to obtain (4.11) for both $f\in C_c^p(\mathbb{R})$ and $f\in\mathfrak{R}_b$. The same approach proves existence of the spectral shift function of order $p\geq 3$ for an unbounded H_0, when $\mathcal{M}=\mathcal{B}(\mathcal{H})$ (the original proofs in [6], [16] were based on the analysis of the Cauchy transform of the measure ν_p). A substantial obstacle in establishing (4.1) for $\tau(|V|^p)<\infty$, with $p>2$ (unless $\tau(|V|^2)<\infty$), is nonextendibility of the set function $m_{p,H_0,V}$ to a finite countably additive measure on $\mathbb{R}^p$ (see a counterexample in [6, Section 4]). An analogous problem has caused a delay in establishing (4.11) in the von Neumann algebra setting; the set function $m_{3,H_0,V}$ can fail to extend to a finite measure even if τ is finite (and $\dim(\mathcal{H}) = \infty$) [6, Section 4]. That is why the approach of [6], [16] working for every Hilbert–Schmidt $V = V^* \in \mathcal{M} = \mathcal{B}(\mathcal{H})$ was not so successful in the general von Neumann algebra setting.

Below we provide an example, which demonstrates that the density η_p, with $p > 3$, reflects information about the shift of the spectrum of an operator H_0 under a perturbation V, similarly to the known case of $p = 2$.

Example. Assume that τ is finite. Let $H_0 = H_0^*$ and $V = V^*$ be commuting operators in $\mathcal{M}$. Then we have the trace formula (4.1) with an absolutely continuous measure $\nu_p \equiv \nu_{p,H_0,V}$, whose density is given by

$$\eta_p(t) = \frac{1}{(p-1)!}\tau\big[(H_0 + V - tI)^{p-1}\big(E_{H_0}(t) - E_{H_0+V}(t)\big)\big] \tag{4.12}$$

$$= \frac{1}{(p-1)!}\tau\big[(H_0 + V - tI)^{p-1}\big(E_{H_0}(t)E_{H_0+V}(t)^\perp - E_{H_0}(t)^\perp E_{H_0+V}(t)\big)\big]. \tag{4.13}$$

Here $E_{H_0}(t)$ denotes the spectral projection $E_{H_0}((-\infty, t))$. If H_0 and $H_0 + V$ are two commuting finite dimensional matrices with the eigenvalues t_k° and t_k, respectively, and τ is the standard trace, then (4.13) computes the net sum of signed powers of distances from t to those eigenvalues t_k, which happen to be on the opposite side of t with the eigenvalues t_k°; the precise formula is

$$\eta_p(t) = \frac{1}{(p-1)!}\sum_{k\in\{k:\ (t_k^\circ - t)(t_k - t)\le 0\}} \big(\mathrm{sign}(t_k - t)\big)(t_k - t)^{p-1}.$$

The representation (4.13) follows directly from (4.12) (see [15, Lemma 2.6]). One can prove existence of an absolutely continuous measure ν_p satisfying (4.1), with the density given by (4.12), by induction on p. In the case of $p = 1$ and $\mathcal{M}$ the algebra of matrices on a finite dimensional Hilbert space, the formula (4.12) is well-known and goes back to [9] and, in the case of a general finite $\mathcal{M}$, it is discussed in [2]. The formula in the case of $p = 2$ is due to [15, Lemma 5.2]. To prove (4.1) and (4.12) for $p > 3$, firstly we note that for ϕ representable in the form (3.1),

$$\int_{\mathbb{R}^{p+1}} \phi(\lambda_1, \lambda_2, \ldots, \lambda_p, \lambda_{p+1})\, dE_{H_1}(\lambda_1)V\, dE_{H_2}(\lambda_2)V \cdots dE_{H_p}(\lambda_p)V\, dE_{H_{p+1}}(\lambda_{p+1})$$
$$= V^p \int_S \alpha_1(H_1, s)\alpha_2(H_2, s)\cdots\alpha_p(H_p, s)\alpha_{p+1}(H_{p+1}, s)\, d\sigma(s).$$

Therefore, the formula (3.2) for the trace of an operator derivative rewrites as

$$\tau\left[\frac{d^p}{dx^p}\bigg|_{x=0} f(H_0+xV)\right] = \int_{\mathbb{R}} f^{(p)}(\lambda)\,d\tau\big[V^p E_{H_0}(\lambda)\big] = \tau\big[V^p f^{(p)}(H_0)\big],$$

for $f \in \mathcal{W}_p(\mathbb{R}) \cup \mathfrak{R}$, and hence,

$$\tau\big[R_{p+1}(f)\big] = \tau\big[R_p(f)\big] - \frac{1}{p!}\tau\big[V^p f^{(p)}(H_0)\big]. \tag{4.14}$$

We suppose that (4.1) holds with $d\nu_p(t) = \eta_p(t)\,dt$, where η_p is given by (4.12), and derive

$$\tau\big[R_{p+1}(f)\big] = \int_{\mathbb{R}} f^{(p+1)}(t)\eta_{p+1}(t)\,dt.$$

Let $H = H_0 + V$. By the binomial theorem we obtain

$$\begin{aligned} &\frac{1}{p!}\tau\big[V^p f^{(p)}(H_0)\big] \\ &\quad= \frac{1}{p!}\tau\big[(H-H_0)^p f^{(p)}(H_0) - (H-H)^p f^{(p)}(H)\big] \\ &\quad= \frac{1}{p!}\sum_{k=0}^{p}\binom{p}{k}(-1)^k\tau\big[H^{p-k}H_0^k f^{(p)}(H_0) - H^{p-k}H^k f^{(p)}(H)\big], \end{aligned} \tag{4.15}$$

which by the spectral theorem can be written as

$$\begin{aligned} &\frac{1}{p!}\sum_{k=0}^{p}\binom{p}{k}(-1)^k\tau\left[H^{p-k}\int_{\mathbb{R}} t^k f^{(p)}(t)\,d\big(E_{H_0}(t)-E_H(t)\big)\right] \\ &\quad= \frac{1}{p!}\sum_{k=0}^{p}\binom{p}{k}(-1)^k\int_{\mathbb{R}} t^k f^{(p)}(t)\,d\tau\big[H^{p-k}\big(E_{H_0}(t)-E_H(t)\big)\big]. \end{aligned} \tag{4.16}$$

Integrating by parts in (4.16) gives

$$\begin{aligned} &\frac{1}{p!}\sum_{k=1}^{p}\binom{p}{k}(-1)^{k+1}k\int_{\mathbb{R}} t^{k-1} f^{(p)}(t)\tau\big[H^{p-k}\big(E_{H_0}(t)-E_H(t)\big)\big]\,dt \\ &\quad+ \frac{1}{p!}\sum_{k=0}^{p}\binom{p}{k}(-1)^{k+1}\int_{\mathbb{R}} t^k f^{(p+1)}(t)\tau\big[H^{p-k}\big(E_{H_0}(t)-E_H(t)\big)\big]\,dt, \end{aligned} \tag{4.17}$$

which by the binomial theorem can be written as

$$\begin{aligned} &\int_{\mathbb{R}} f^{(p)}(t)\frac{1}{(p-1)!}\tau\big[(H-tI)^{p-1}\big(E_{H_0}(t)-E_H(t)\big)\big]\,dt \\ &\qquad- \int_{\mathbb{R}} f^{(p+1)}(t)\frac{1}{p!}\,d\tau\big[(H-tI)^p\big(E_{H_0}(t)-E_H(t)\big)\big]\,dt. \end{aligned} \tag{4.18}$$

By the induction hypothesis, the first summand in (4.18) equals $\tau[R_p(f)]$. Thus, combining (4.14)–(4.18) completes the proof of (4.12).

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