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Differentiation, Taylor series, and all order spectral shift functions, for relatively bounded perturbations

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Given H self-adjoint, V symmetric and relatively H-bounded, and $f : \mathbb{R} \to \mathbb{C}$ satisfying mild conditions, we show that the Gateaux derivative

$$\frac{d^n}{dt^n} f(H+tV)|_{t=0}$$

exists in the operator norm topology, for every natural n, and establish perturbation formulas for multiple operator integrals under relatively bounded perturbations. If the H-bound of V is less than 1, we obtain sufficient conditions on f which ensure that the Taylor expansion

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

exists and converges absolutely in operator norm. Assuming that $V(H-i)^{-p} \in \mathcal{S}^{s/p}$ for $p = 1, \dots, s$ for some $s \in \mathbb{N}$, we show that the Krein–Koplienko spectral shift functions $\eta_{k,H,V}$, satisfying

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$$\mathrm{Tr}\left(f(H+V)-\sum_{m=0}^{k-1}\frac{1}{m!}\frac{d^m}{dt^m}f(H+tV)\big|_{t=0}\right)$$
$$=\int_{\mathbb{R}} f^{(k)}(x)\eta_{k,H,V}(x)dx,$$

exist for every $k = 1,2,3,\ldots$, independently of s. The latter result (which is significantly stronger than [27]) is new also in the case that V is bounded. The proof is based on [34], combined with a generalisation of the multiple operator integral compatible with [17]. We discuss applications of our results to quantum physics and noncommutative geometry.

1. Introduction

The Taylor series is a fundamental tool in real analysis, and its noncommutative or operator-theoretic generalization is useful in quantum mechanics, quantum field theory, and noncommutative geometry. It relies firstly on the existence of derivatives of operator functions, for which the most natural setting is arguably the one of Kato and Rellich. Indeed, if H is a self-adjoint (possibly unbounded) operator in a separable Hilbert space $\mathcal{H}$, and V is symmetric and relatively H-bounded, then the Kato–Rellich theorem states that

$$H+tV \qquad \text{is self-adjoint for all} \qquad t\in(-\tfrac{1}{a},\tfrac{1}{a}),$$

where a is the H-bound of V. Hence, by Borel functional calculus, we may apply a bounded measurable function $f:\mathbb{R}\to\mathbb{C}$ to obtain a mapping

$$(-\tfrac{1}{a},\tfrac{1}{a})\to\mathcal{B}(\mathcal{H}),\qquad t\mapsto f(H+tV). \tag{1}$$

For suitable classes of f, the following questions may arise:

- Q1. Is $t\mapsto f(H+tV)$ n-times differentiable?
- Q2. Does the Taylor-expansion of $f(H+tV)$ in orders of t converge in norm?
- Q3. Do all higher-order spectral shift functions exist?

For reasons of summability, more assumptions on H and V are needed to affirmatively answer Q3, as detailed in the next subsection. It turns out that Q1 and Q2 have an affirmative answer without extra assumptions on H and V, and with conditions on f that are relatively easy to verify.

Pioneering results concerning the differentiability of the operator function (1) were obtained in [11] by use of the *double operator integral.* The n-th order derivative of the operator function (1), for bounded perturbations V, is naturally expressed in terms of a *multiple operator integral* (a concept originating in [5,11,31,44,45]), which generalizes the notion of a double operator integral to more than two variables (see, e.g., [4,7,17,32,34–36, 41]). A series of works has since addressed the differentiability of such operator functions under various conditions on f, H, and V – see [43, Paragraph 5.3], and references therein.

When differentiating in the direction of an unbounded operator V, the operator-norm Frechet derivative of (1) is useless because it contains $\|V\| = \infty$ in the denominator. One is thus led to the Gateaux derivative, for which the following holds.

Theorem 1. *Let H be self-adjoint in a separable Hilbert space $\mathcal{H}$, and let V be symmetric and relatively H-bounded with H-bound $a \in [0, \infty)$. If $n \in \mathbb{N}$ and $f \in C^{n+1}(\mathbb{R})$ is such that the functions $\frac{d^p}{dx^p}(f(x)(x-i)^p)$ are Fourier transforms of finite complex measures for all $p = 0, \ldots, n+1$, then the mapping*

$$(-\tfrac{1}{a}, \tfrac{1}{a}) \to \mathcal{B}(\mathcal{H}), \qquad t \mapsto f(H + tV)$$

is n times differentiable in operator norm.

The above result follows from Theorem 22, which moreover provides alternative conditions to ensure operator differentiability, and establishes that

$$\frac{1}{n!}\frac{d^n}{dt^n} f(H + tV)\big|_{t=0} = \mathbf{T}^{H,\ldots,H}_{f^{[n]}}(V, \ldots, V), \tag{2}$$

in which $\mathbf{T}^{H,\ldots,H}_{f^{[n]}}$ is an n-multilinear map from relatively bounded operators to bounded operators which extends the multiple operator integral of [4,32] and is compatible with [17]. The main reason multiple operator integrals are powerful tools in perturbation theory, noncommutative analysis, and noncommutative geometry, is because of their surprisingly clean analytical and algebraic properties. We extend several such properties to the relatively bounded setting. A further motivation for these developments are the questions raised in [48].

For unbounded V, trying to obtain (2) directly by naively extending the multiple operator integral (directly inserting V in the integral) fails because of domain problems. The intuition behind a formula like (2) in the relatively bounded setting is that the summability of a multiple operator integral $T^{H,\ldots,H}_{\phi}(V, \ldots, V)$ is typically related to the asymptotic behaviour of its symbol ϕ, and for suitable f the asymptotic behaviour of the divided difference $f^{[n]}(\lambda_0, \ldots, \lambda_n)$ can be controlled by $\lambda_0^{-1} \cdots \lambda_n^{-1}$. In the unbounded case however, distinct subtleties arise in the translation from symbols to operators, which we address with combinatorial techniques.

The results mentioned above yield explicit expressions and bounds for the higher-order operator-norm Gateaux derivative $\frac{d^n}{dt^n} f(H + tV)\big|_{t=0}$ and the Taylor remainder. Particular upshots are algebraic rules for multi-variable Gateaux derivatives (see Remark 23), and the existence of a constant c_f such that

$$\|f(H+V)-f(H)\| \leq c_f \|V(H-i)^{-1}\|.$$

It would be interesting if the same techniques, or some modified version of them, could be used to obtain optimal constants.

Using Theorem 1, we establish the existence of an absolutely norm-converging Taylor series. The respective radius of convergence is related both to $\|V(H-i)^{-1}\|$ and an explicit norm of f, which uses the smoothness as well as the decay at infinity of f.

Theorem 2. *Let H be self-adjoint in a separable Hilbert space $\mathcal{H}$, and let V be symmetric and relatively H-bounded with H-bound $a \in [0,1)$. Let $f \in C^\infty(\mathbb{R})$ be such that $\frac{d^n}{dx^n}(f(x)(x-i)^n)$ are Fourier transforms of finite complex measures μ_n for all $n \in \mathbb{N}$ and let there exist constants $c_f, C_f > 0$ such that $\|\mu_n\| \leq c_f C_f^n n!$ (see Lemma 25 for examples). If $\|V(H-i)^{-1}\| < \frac{1}{1+C_f}$, then we have*

$$f(H+V) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n}{dt^n} f(H+tV)\big|_{t=0},$$

where the series converges absolutely in operator norm. If $\|\mu_n\| \leq c_f C_f^n (n!)^\gamma$ for $\gamma < 1$ then the above identity holds, with absolutely norm-converging series, without any assumption on $\|V(H-i)^{-1}\|$.

The 'noncommutative Taylor series' may be understood as the combination of Theorem 2 and (2), possibly supplemented with one of the various explicit (integral) expressions for (2). As such, the noncommutative Taylor series has been studied in numerous contexts [13,17,24,10,16,15]. In quantum physics it often comes in guises such as the Dyson series, Volterra series and Born series. In noncommutative geometry, the noncommutative Taylor series comes up in the context of the spectral action [40,46,29] and heat kernel expansions [24,19,17], and the algebraic structure underlying its summands can be informative [30]. We hope that, by unifying results scattered throughout the literature, Theorem 2 and (2) bring connections between these applications to the foreground.

Spectral shift functions of all orders. The spectral shift function is a useful notion for the spectral analysis of quantum systems, and the question of its existence has sparked enormous progress in mathematical perturbation theory. First defined by Krein [23], and generalized to higher order by Koplienko [22], the spectral shift function of order k is the function $\eta_k = \eta_{H_0,V,k}$ such that for all sufficiently regular $f : \mathbb{R} \to \mathbb{C}$ we have

$$\operatorname{Tr}\left(f(H+V) - \sum_{m=0}^{k-1} \frac{d^m}{dt^m} f(H+tV)\big|_{t=0} \right) = \int_{\mathbb{R}} \eta_k(x) f^{(k)}(x)dx.$$

In [34] the spectral shift functions η_k of orders $k \geq n$ were shown to exist whenever $V \in \mathcal{S}^n$. Because physical situations – for example when H is a differential operator and V a multiplication operator – require V to have continuous spectrum, the paper [27] used the much weaker assumption $V(H-i)^{-1} \in \mathcal{S}^n$ $(n \in \mathbb{N})$ to obtain the spectral shift functions of order $k \geq n$. Under a similar assumption, [28] added existence of η_{n-1} when n is even. Throughout the literature one finds many such assumptions which generalise the case of $(H-i)^{-1} \in \mathcal{S}^n$ to a 'locally compact' setting. Often, existence of the spectral shift function depends on n, which for a differential operator H depends on its order and the dimension of the underlying space. The notable exception is that η_1 was shown to exist independently of n in [50]. However, for general $n \in \mathbb{N}$, existence of $\eta_2, \ldots, \eta_{n-1}$ remained open, even for bounded V and under any of the above reasonable conditions.

The final result of this paper is the existence, uniqueness and regularity properties of η_k for all orders $k \in \mathbb{N}$ under the assumptions that V is symmetric and

$$V(H-i)^{-p} \in \mathcal{S}^{n/p} \qquad (p = 1, \ldots, n), \tag{3}$$

for an arbitrary $n \in \mathbb{N}$. The assumption (3) unifies the 'locally compact' assumption $V(H-i)^{-n} \in \mathcal{S}^1$ with the 'relative Schatten' assumption $V(H-i)^{-1} \in \mathcal{S}^n$ and is used in [38,42,47]. We exemplify its applicability in Section 6.1.

In practice, the summability n should be correlated with the dimension of the underlying space and the order of the initial differential operator. The fact that in [28] this summability is correlated with the order of the spectral shift function, is thus revealed as an artefact from not starting with the 'right' assumption.

Similar but distinct from the above crucial point, the boundedness assumption on V appearing in previous works is revealed to be artificial by Theorem 40. This shows the power of our extension of the multiple operator integral and the superscript difference identity, Theorem 16.

Compared to earlier results on higher-order spectral shift [34,27,28], the proof moreover gains an inductive structure: existence of the spectral shift function η_k can be deduced from the existence of η_{k-1}. Our proof is thus split into induction basis – existence of η_1 – in Section 5.1, and induction step in Section 5.2. Under different assumptions, existence of η_1 was already known, and the reader only interested in the cases already covered by [50] needs only to read Section 5.2.

While finishing this manuscript, the authors became aware of the preprint version of [2], which independently obtains first-order differentiability for relatively bounded perturbations and a sharpening of [50] for relatively trace-class perturbations, for a different class of scalar functions. During the review process of the current paper, an independent preprint [14] appeared connecting higher-order spectral shift functions with index theory for a concrete class of operators; its use of multiple operator integrals is closely related to our approach, though the goals differ.

This article is structured as follows. Section 2 contains preliminaries, Section 3 proves the multiple operator integration techniques needed in Sections 4 and 5, Section 4 proves higher-order differentiability and existence of Taylor series, and Section 5 studies the existence of spectral shift functions of all orders.

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2. Preliminaries

Notations and conventions. We write $\mathbb{N} = \{1, 2, ...\}$. We let $\mathcal{H}$ be a separable Hilbert space, and $\mathcal{B}(\mathcal{H})$ the bounded linear operators on $\mathcal{H}$. For $p \in [1, \infty)$, we let $\mathcal{S}^p = \mathcal{S}^p(\mathcal{H})$ denote the Banach space of Schatten p-class operators, with the Schatten norm $\| \cdot \|_p$. We use the convention that $\mathcal{S}^\infty = \mathcal{S}^\infty(\mathcal{H})$ denotes the set of all compact operators on $\mathcal{H}$ with the usual operator norm $\|A\|_\infty = \|A\|$. By "H is self-adjoint in $\mathcal{H}$" we mean H is a self-adjoint possibly unbounded operator on a (dense) domain $\mathrm{dom}(H) \subseteq \mathcal{H}$. We use the convention that $(-\frac{1}{a}, \frac{1}{a}) = (-\infty, \infty)$ if $a = 0$. We define $u : \mathbb{R} \to \mathbb{C}$ by

$$u(x) := x - i.$$

Let X be an interval in $\mathbb{R}$ possibly coinciding with $\mathbb{R}$. Let $C(X)$ denote the space of all continuous functions on X, $C_0(\mathbb{R})$ the space of continuous functions on $\mathbb{R}$ decaying to 0 at infinity, $C^n(X)$ the space of n-times continuously differentiable functions on X. Let $C_b^n(X)$ denote the subset of $C^n(X)$ of such f for which $f^{(n)}$ is bounded. Let $C_c^n(\mathbb{R})$ denote the subspace of $C^n(\mathbb{R})$ consisting of compactly supported functions. We also use the notation $C^0(\mathbb{R}) = C(\mathbb{R})$. Let $C_c^n(X)$ denote the subspace of $C_c^n(\mathbb{R})$ consisting of the functions whose closed support is contained in X. For $p \in [1, \infty]$, let $L^p(\mathbb{R})$ denote the Lebesgue L^p-space with usual norm $\|f\|_p = \|f\|_{L^p(\mathbb{R})}$. Let $L^1_{\mathrm{loc}}(\mathbb{R})$ denote the space of functions locally integrable on $\mathbb{R}$ equipped with the seminorms $f \mapsto \int_{-a}^{a} |f(x)|\, dx$, $a > 0$. For any $f \in L^1(\mathbb{R})$, $\hat{f}$ denotes the Fourier transform with convention $f(x) = \int_{\mathbb{R}} \hat{f}(y) e^{ixy} dx$. We canonically extend this Fourier transform to tempered distributions, though any distribution that we shall encounter in this paper will be canonically represented by a function or a measure. For a finite measure μ we write $\|\mu\|$ for its total variation, which coincides with the corresponding L^1-norm if μ is absolutely continuous.

2.1. New function spaces

Let $n \in \mathbb{Z}_{\geq 0}$. We introduce the following function spaces:

$$W_0(\mathbb{R}) := \{f \in C_b(\mathbb{R}) : \ f(x) = \int_{\mathbb{R}} e^{ixy} d\mu(y) \text{ for a finite complex measure } \mu \text{ on } \mathbb{R}\},$$

$$\mathscr{W}_n(\mathbb{R}) := \{f \in C^n(\mathbb{R}) : \ (fu^p)^{(p)} \in W_0(\mathbb{R}), \ p = 0, \ldots, n\}.$$

For each $k \leq n$ we also introduce the auxiliary space:

$$\begin{aligned}\mathscr{W}_k^n(\mathbb{R}) &= \{f \in C^n(\mathbb{R}) : \ (fu^p)^{(n-k+p)} \in W_0(\mathbb{R}), p = 0, \ldots, k\} \\ &= \{f \in C^n(\mathbb{R}) : \ (fu^{k-n+p'})^{(p')} \in W_0(\mathbb{R}), p' = n-k, \ldots, n\}.\end{aligned}$$

The following lemma shows that test functions such as rational functions, Schwartz class functions, and $C_c^{n+1}(\mathbb{R})$ are contained in the newly introduced function classes.

Lemma 3. *Let $n \in \mathbb{N}$. Then, the following assertions hold.*

(a) *For every $\alpha > \frac{1}{2}$,*

$$\left\{f \in C^{n+1}(\mathbb{R}) : \ f^{(p)}(x) = \mathcal{O}\left(|x|^{-p-\alpha}\right) \ \text{as } |x| \to \infty, \ p = 0, \ldots, n+1\right\} \subseteq \mathscr{W}_n(\mathbb{R}).$$

(b) *For each $k \leq n$ and for every $\alpha > \frac{1}{2}$,*

$$\begin{aligned}&\{f \in C^{n+1}(\mathbb{R}) : \ f^{(p)}(x) = \mathcal{O}\left(|x|^{-p+n-k-\alpha}\right) \\ &\qquad \text{as } |x| \to \infty, \ p = n-k, \ldots, n+1\} \subseteq \mathscr{W}_k^n(\mathbb{R}).\end{aligned}$$

Proof. By [33, Lemma 7], we have the implications

$$f \in L^2(\mathbb{R}) \cap C^1(\mathbb{R}), \ f' \in L^2(\mathbb{R}) \quad \Rightarrow \quad \hat{f} \in L^1(\mathbb{R}) \quad \Rightarrow \quad f \in W_0(\mathbb{R}), \tag{4}$$

from which the lemma follows after applying the repeated Leibniz rule. □

Let us collect some further properties of these function spaces.

Lemma 4. *For $n, k \in \mathbb{N}$, $k \leq n$, $p \in \mathbb{Z}_{\geq 0}$, the following holds.*

(a) *If $f \in \mathscr{W}_k^n(\mathbb{R})$ then $fu \in \mathscr{W}_{k-1}^n(\mathbb{R})$ and $f \in \mathscr{W}_{k-1}^{n-1}(\mathbb{R})$.*
(b) *If $(fu^p)^{(n)} \in W_0(\mathbb{R})$ and $(fu^{p+1})^{(n+1)} \in W_0(\mathbb{R})$ then $(fu^p)^{(n+1)} \in W_0(\mathbb{R})$.*
(c) *We have $\mathscr{W}_n(\mathbb{R}) = \{f \in C^n(\mathbb{R}) : \ (fu^p)^{(m)} \in W_0(\mathbb{R}) \ \text{ for } \ 0 \leq p \leq m \leq n\}$.*

Proof. The first statement follows by definition of $\mathscr{W}_k^n(\mathbb{R})$.

We proceed to the second statement. As $u' = 1$, $u'' = 0$, we have

$$(fu^{p+1})^{(n+1)} = (fu^p)^{(n+1)}u + (n+1)(fu^p)^{(n)}.$$

Therefore,

$$(fu^p)^{(n+1)} = (fu^{p+1})^{(n+1)}u^{-1} - (n+1)(fu^p)^{(n)}u^{-1}. \tag{5}$$

The Fourier transform of u^{-1} is in $L^1(\mathbb{R})$ because $u^{-1}, (u^{-1})' \in C^\infty(\mathbb{R}) \cap L^2(\mathbb{R})$ and we may apply (4). Hence, $u^{-1} \in W_0(\mathbb{R})$, and because $W_0(\mathbb{R})$ is an algebra (the convolution of complex measures is a complex measure), the second statement of the lemma follows from (5).

The third statement is a straightforward consequence of the second. $\square$

2.2. Relative boundedness

Definition 5. Let H be self-adjoint in $\mathcal{H}$. A linear operator V with domain $\operatorname{dom} V \subseteq \mathcal{H}$ is called (relatively) H-bounded if $\operatorname{dom} H \subseteq \operatorname{dom} V$ and there exist $a, b \in [0, \infty)$ such that for all $\psi \in \operatorname{dom} H$ we have

$$\|V\psi\| \leq a\,\|H\psi\| + b\,\|\psi\|\,.$$

The infimum over such numbers a is called the H-bound of V.

We collect the following properties of relatively bounded operators.

Lemma 6. *Let H be self-adjoint in $\mathcal{H}$.*

(a) *If V is relatively H-bounded with H-bound a, then $V(H-i)^{-1} : \mathcal{H} \to \mathcal{H}$ is bounded, and $a \leq \|V(H-i)^{-1}\| \leq a + b$.*
(b) *If V is relatively H-bounded with H-bound a, then for all $z \in \mathbb{C}$ the operator zV is relatively H-bounded with H-bound $|z|a$.*
(c) *The space of relatively H-bounded operators is a $\mathbb{C}$-vector space and a left $\mathcal{B}(\mathcal{H})$-module for the canonical addition, scalar multiplication, and multiplication of operators in $\mathcal{H}$.*
(d) *If V is symmetric and relatively H-bounded with H-bound a then*

$$H + tV \quad \text{is self-adjoint on} \quad \operatorname{dom}(H + tV) = \operatorname{dom}(H)$$

for all $t \in (-\frac{1}{a}, \frac{1}{a})$.
(e) *If V is symmetric and relatively H-bounded with H-bound a, then V is relatively $H+tV$-bounded for all $t \in (-\frac{1}{a}, \frac{1}{a})$ with $H+tV$-bound $\leq \frac{a}{1-|t|a}$. Moreover, $\|V(H + tV - i)^{-1}\| \leq \frac{a+b}{1-|t|a}$.*

Proof. Statements (a), (b), and (c) follow directly from Definition 5. Statement (d) follows from the Kato–Rellich theorem [20, Theorem V-4.3] (originally proved by Rellich) combined with (a). From the triangle inequality applied to $\|V\psi\| \leq a\|(H+tV)\psi - tV\psi\| + b\|\psi\|$, it follows that

$$\|V\psi\| \leq \frac{a}{1-a|t|}\|(H+tV)\psi\| + \frac{b}{1-a|t|}\|\psi\|.$$

The final statement of (e) thus follows from (a) which by (d) applies to $H + tV$ instead of H. □

We shall make plenty use of the second resolvent identity, which conveniently also holds in the relatively bounded setting. See also the version for closed operators, cf. [6, Lemma 2].

Lemma 7 *(second resolvent identity). Let H be self-adjoint and let V be symmetric and relatively H-bounded with H-bound < 1. For each $z \in \mathbb{C}$ with $Im\ z \neq 0$, we have*

$$(H + V - z)^{-1} - (H - z)^{-1} = -(H + V - z)^{-1}V(H - z)^{-1}.$$

Proof. After noting that $H + V$ is self-adjoint on $\mathrm{dom}(H + V) = \mathrm{dom}(H)$ (see Lemma 6(d)), the proof is the same as in the bounded case. □

3. Multiple operator integrals with relatively bounded arguments

We generalize the multiple operator integral to relatively bounded arguments, and analyze its algebraic and analytical properties. The construction is inspired by, and compatible with, [17] and [1].

We first recall the definition of the multiple operator integral for bounded arguments, as given in [4,32]. For an overview, see [43].

Definition 8. Let $n \in \mathbb{N}$, let $H_0, \ldots, H_n$ be self-adjoint in $\mathcal{H}$, and let $V_1, \ldots, V_n \in \mathcal{B}(\mathcal{H})$. For a function $\phi : \mathbb{R}^{n+1} \to \mathbb{C}$, we write $\phi \in \mathfrak{BS}(\mathbb{R}^{n+1})$ (or $\phi \in \mathfrak{BS}$ for short) if there exist a finite[1] measure space $(\Omega, d\omega)$ and bounded measurable functions $a_0, \ldots, a_n : \mathbb{R} \times \Omega \to \mathbb{C}$ such that

$$\phi(\lambda_0, \ldots, \lambda_n) = \int_\Omega a_0(\lambda_0, \omega) \cdots a_n(\lambda_n, \omega)\, d\omega. \tag{6}$$

If ϕ is of the above form, then the multiple operator integral (MOI) $T_\phi^{H_0,\ldots,H_n}$ is defined by

[1] It is equivalent to use σ-finite measure spaces under a condition on the norms of $a_i(\cdot, \omega)$, see [43, p.48] (and [17, Lemma 2.5]).

$$T_\phi^{H_0,\ldots,H_n}(V_1,\ldots,V_n)\psi := \int_\Omega a_0(H_0,\omega)V_1 a_1(H_1,\omega)\cdots V_n a_n(H_n,\omega)\psi\, d\omega \qquad (\psi\in\mathcal{H}),$$

in which the right-hand side is a Bochner integral.

It follows that the operator $T_\phi^{H_0,\ldots,H_n} : \mathcal{B}(\mathcal{H})\times\cdots\times\mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ is well-defined and bounded. Importantly, the operator $T_\phi^{H_0,\ldots,H_n}$ depends only on ϕ, not on the measure space $(\Omega, d\omega)$ or the functions a_j [4, Lemma 4.3]. The following extension of the MOI to unbounded arguments is simple but surprisingly powerful, and will be the main tool of this paper.

Definition 9. Let $n\in\mathbb{Z}_{\geq 0}$, let $H_0,\ldots,H_n$ be self-adjoint in $\mathcal{H}$, and let V_j be relatively H_j-bounded for $j=1,\ldots,n$. Let $\alpha=(\alpha_1,\ldots,\alpha_n)\in\mathbb{Z}^n_{\geq 0}$ be such that $V_j(H_j-i)^{-\alpha_j}\in\mathcal{B}(\mathcal{H})$, and define $u^\alpha := u_1^{\alpha_1}\cdots u_n^{\alpha_n}$, where $u_j(\lambda_0,\ldots,\lambda_n):=\lambda_j - i$. For any measurable $\phi:\mathbb{R}^{n+1}\to\mathbb{C}$ such that $\phi u^\alpha\in\mathfrak{BS}(\mathbb{R}^{n+1})$ we define the multiple operator integral with relatively bounded arguments as

$$\mathbf{T}_\phi^{H_0,\ldots,H_n}(V_1,\ldots,V_n) := T_{\phi u^\alpha}^{H_0,\ldots,H_n}(V_1(H_1-i)^{-\alpha_1},\ldots,V_n(H_n-i)^{-\alpha_n}). \tag{7}$$

Lemma 10. *Definition 9 is well-defined, and for all $V_1,\ldots,V_n\in\mathcal{B}(\mathcal{H})$ we have*

$$\mathbf{T}_\phi^{H_0,\ldots,H_n}(V_1,\ldots,V_n) = T_\phi^{H_0,\ldots,H_n}(V_1,\ldots,V_n),$$

where $n\in\mathbb{N}$, $H_0,\ldots,H_n$ are self-adjoint, and $\phi\in\mathfrak{BS}(\mathbb{R}^{n+1})$.

Proof. Let $\alpha,\beta\in\mathbb{Z}^n_{\geq 0}$ be such that $V_j(H_j-i)^{-\alpha_j}$ is bounded for all j. Then, $V_j(H_j-i)^{-\alpha_j-\beta_j}$ is bounded as well. Moreover, it follows from Definition 8 that

$$\begin{aligned}&T_{\phi u^{\alpha+\beta}}^{H_0,\ldots,H_n}(V_1(H_1-i)^{-\alpha_1-\beta_1},\ldots,V_n(H_n-i)^{-\alpha_n-\beta_n})\\ &= T_{\phi u^\alpha}^{H_0,\ldots,H_n}(V_1(H_1-i)^{-\alpha_1},\ldots,V_n(H_n-i)^{-\alpha_n}).\end{aligned}$$

Hence, the right-hand side of (7) is independent from α, yielding the first statement of the lemma. Taking $\alpha=(0,\ldots,0)$ yields the second. □

An important special case of Definition 9 is obtained when the symbol ϕ is a divided difference $\phi=f^{[n]}$ of a function $f\in C^n(\mathbb{R})$. The divided difference is defined recursively by

$$\begin{aligned}f^{[0]}(\lambda) &:= f(\lambda),\\ f^{[n]}(\lambda_0,\ldots,\lambda_n) &:= \frac{f^{[n-1]}(\lambda_0,\ldots,\lambda_{n-1}) - f^{[n-1]}(\lambda_1,\ldots,\lambda_n)}{\lambda_0-\lambda_n},\end{aligned}$$

where the fraction is continuously extended when $\lambda_0=\lambda_n$. We shall moreover use the following alternate representation of $f^{[n]}$.

Lemma 11. *Let $f \in C^n(\mathbb{R})$ such that $f^{(n)} \in W_0(\mathbb{R})$, with $f^{(n)}(\lambda) = \int e^{ix\lambda} d\mu(x)$. Then, for all $\lambda_0, \dots, \lambda_n \in \mathbb{R}$,*

$$f^{[n]}(\lambda_0, \dots, \lambda_n) = \int_{\mathbb{R}} \int_{\Delta_n} e^{is_0 x \lambda_0} e^{is_1 x \lambda_1} \cdots e^{is_n x \lambda_n} \, ds \, d\mu(x),$$

where the simplex $\Delta_n = \{s = (s_0, \dots, s_n) \in \mathbb{R}^{n+1}_{\geq 0} \ : \ s_0 + \dots + s_n = 1\}$ is endowed with the flat measure with total measure $1/n!$. Clearly, $(\mathbb{R} \times \Delta_n, d\mu(x) \times ds)$ is a finite measure space, hence $f^{[n]} \in \mathfrak{BS}$.

Proof. The proof follows directly from the arguments presented in [34, Lemmas 5.1 and 5.2]. □

Corollary 12. *Let $n \in \mathbb{N}$, $H_0, \dots, H_n$ be self-adjoint operators in $\mathcal{H}$ and let $f \in C^n(\mathbb{R})$ be such that $f^{(n)} \in W_0(\mathbb{R})$, $f^{(n)}(\lambda) = \int e^{ix\lambda} d\mu(x)$. For all $V_1, \dots, V_n \in \mathcal{B}(\mathcal{H})$ and all $\psi \in \mathcal{H}$ we have*

$$T^{H_0, \dots, H_n}_{f^{[n]}}(V_1, \dots, V_n)\psi = \int_{\mathbb{R}} \int_{\Delta_n} e^{is_0 x H_0} V_1 e^{is_1 x H_1} \cdots V_n e^{is_n x H_n} \psi \, ds \, d\mu(x).$$

Consequently, for all $\alpha, \alpha_j \in [1, \infty]$ with $\frac{1}{\alpha_1} + \dots + \frac{1}{\alpha_n} = \frac{1}{\alpha}$,

$$\big\| T^{H_0, \dots, H_n}_{f^{[n]}} \big\|_{\mathcal{S}^{\alpha_1} \times \dots \times \mathcal{S}^{\alpha_n} \to \mathcal{S}^{\alpha}} \leq \frac{1}{n!} \big\| \mu \big\|. \tag{8}$$

Proof. Combining Definition 8 with Lemma 11, and using $\phi = f^{[n]}$, the corollary follows. □

The following theorem explains the power of Definition 9.

Theorem 13. *For $n \in \mathbb{N}$, $H_0, \dots, H_n$ self-adjoint in $\mathcal{H}$, and $f \in \mathscr{W}_n(\mathbb{R})$, we have $f^{[n]} u^{(1, \dots, 1)} \in \mathfrak{BS}(\mathbb{R}^{n+1})$, and hence Definition 9 defines a multilinear map*

$$\mathbf{T}^{H_0, \dots, H_n}_{f^{[n]}} : \mathbf{X}_{H_1} \times \dots \times \mathbf{X}_{H_n} \to \mathcal{B}(\mathcal{H}),$$

where $\mathbf{X}_H$ is the space of H-bounded operators (which is a linear space by Lemma 6(c)). More generally, if $\alpha = (\alpha_1, \dots, \alpha_n) \in \{0, 1\}^n$ is such that $V_j \in \mathcal{B}(\mathcal{H})$ if $\alpha_j = 0$, and $f \in \mathscr{W}^n_{|\alpha|}(\mathbb{R})$, then $f^{[n]} u^{\alpha} \in \mathfrak{BS}(\mathbb{R}^{n+1})$, and hence Definition 9 defines a multilinear map

$$\mathbf{T}^{H_0, \dots, H_n}_{f^{[n]}} : \mathbf{X}^{\alpha_1}_{H_1} \times \dots \times \mathbf{X}^{\alpha_n}_{H_n} \to \mathcal{B}(\mathcal{H}),$$

where $\mathbf{X}^1_H = \mathbf{X}_H$ and $\mathbf{X}^0_H = \mathcal{B}(\mathcal{H})$.

Proof. The first statement of the theorem follows by combining Lemma 11 with the formula

$$f^{[n]}(\lambda_0,\dots,\lambda_n) = \sum_{p=0}^{n}(-1)^{n-p}\sum_{0<j_1<\dots<j_p\le n}(fu^p)^{[p]}(\lambda_0,\lambda_{j_1},\dots,\lambda_{j_p})u^{-1}(\lambda_1)\cdots u^{-1}(\lambda_n), \tag{9}$$

which was shown in [27, Eq. (24)]. Let $\mathcal{J}=\{j\in\{1,\dots,n\} : \alpha_j=1\}$, and $\mathcal{J}^{\mathrm{c}}=\{1,\dots,n\}\setminus\mathcal{J}$. The second statement of the theorem follows by combining Lemma 11 with the formula

$$f^{[n]}(\lambda_0,\dots,\lambda_n) = \sum_{p=n-|\alpha|}^{n}(-1)^{n-p}\sum_{\substack{0<j_1<\dots<j_p\le n\\ \{j_1,\dots,j_p\}\supseteq\mathcal{J}^{\mathrm{c}}}}(fu^{n-|\alpha|+p})^{[p]}(\lambda_0,\lambda_{j_1},\dots,\lambda_{j_p})\prod_{j\in\mathcal{J}}u^{-1}(\lambda_j),$$

which can be shown in a similar way (see [28, eq. (21)]). □

3.1. Perturbation formulas for the generalised multiple operator integral

It turns out that several useful identities of the multiple operator integral extend to the case of relatively bounded arguments. In order not to interrupt the flow of the paper, their proofs are in the appendix.

The first such identity is a change of variables rule which adds resolvents of the superscript operators to the arguments. This identity forms a key step in deriving summability estimates for multiple operator integrals, as witnessed in the bounded case by [9,27–29], and in the relatively bounded case in Sections 4 and 5.

Theorem 14 *(change-of-variables). Let $H_0,\dots,H_n$ be self-adjoint in $\mathcal{H}$. Let $\mathcal{J}\subseteq\{1,\dots,n\}$ be a subset so that V_k is bounded for each $k\in\{1,\dots,n\}\setminus\mathcal{J}$ and V_k is relatively H_k-bounded for each $k\in\mathcal{J}$. For each $f\in\mathcal{W}^n_{|\mathcal{J}|}(\mathbb{R})$ and each $j\in\{0,1,\dots,n\}$ (the boundary cases $j=0$ and $j=n$ being understood as in Theorem 47) we have*

$$\begin{aligned}\mathbf{T}^{H_0,\dots,H_n}_{f^{[n]}}(V_1,\dots,V_n) &= \mathbf{T}^{H_0,\dots,H_n}_{(fu)^{[n]}}(V_1,\dots,V_{j-1},V_j(H_j-i)^{-1},V_{j+1},\dots,V_n)\\ &\quad - \mathbf{T}^{H_0,\dots,H_{j-1},H_{j+1},\dots,H_n}_{f^{[n-1]}}(V_1,\dots,V_{j-1},V_j(H_j-i)^{-1}V_{j+1},V_{j+2},\dots,V_n).\end{aligned}$$

Proof. Follows from Theorem 48 in the appendix. □

By repeating the proof of the above change of variables rule, one expands a generalised multiple operator integral into a finite sum of multiple operator integrals with bounded arguments. This in particular generates a useful norm bound of the (generalised) multiple operator integral.

Theorem 15. *Let $n \in \mathbb{N}$, let $H_0, \dots, H_n$ be self-adjoint in $\mathcal{H}$. For each $j \in \{1, \dots, n\}$, let V_j be a relatively H_j-bounded operator. Let $f \in \mathscr{W}_n(\mathbb{R})$ (i.e., $f \in C^n(\mathbb{R})$ such that $(fu^p)^{(p)} \in W_0(\mathbb{R})$ for all $p \in \{0, \dots, n\}$). Writing $\tilde{V}_{j,l} := V_{j+1}(H_{j+1} - i)^{-1} \cdots V_l(H_l - i)^{-1} \in \mathcal{B}(\mathcal{H})$, we have*

$$\mathbf{T}^{H_0,\dots,H_n}_{f^{[n]}}(V_1, \dots, V_n) = \sum_{p=0}^{n} (-1)^{n-p} \sum_{0<j_1<\dots<j_p\le n} T^{H_0,H_{j_1},\dots,H_{j_p}}_{(fu^p)^{[p]}}(\tilde{V}_{0,j_1}, \dots, \tilde{V}_{j_{p-1},j_p})\tilde{V}_{j_p,n}\,.$$

Here, the case $p = 0$ on the right-hand side of the above identity is understood as $f(H_0)\tilde{V}_{0,n}$. Therefore, if $\widehat{(fu^p)^{(p)}} \in L^1(\mathbb{R})$ we have

$$\left\|\mathbf{T}^{H_0,\dots,H_n}_{f^{[n]}}(V_1, \dots, V_n)\right\| \le \sum_{p=0}^{n} \binom{n}{p} \frac{1}{p!} \left\|\widehat{(fu^p)^{(p)}}\right\|_1 \prod_{j=1}^{n} \left\|V_j(H_j - i)^{-1}\right\|,$$

and if $\widehat{(fu^p)^{(p)}} \notin L^1$ then $\|\widehat{(fu^p)^{(p)}}\|_1$ may be replaced by $\|\mu_p\|$, where $(fu^p)^{(p)}(x) = \int e^{ixy} d\mu_p(y)$.

Proof. The first identity follows from repeated application of Theorem 14 and Lemma 10. The bound follows from Corollary 12. □

The following superscript difference identity is crucial for calculating derivatives and Taylor series. The proof is surprisingly subtle.

Theorem 16. *Let $n \in \mathbb{N}$, let $H_0, \dots, H_n$ be self-adjoint in $\mathcal{H}$, and let $f \in \mathscr{W}_{n+1}(\mathbb{R})$. For each $j \in \{1, \dots, n\}$, let V_j be a H_j-bounded symmetric operator with H_j-bound a. For all $t \in (-\frac{1}{a}, \frac{1}{a})$ and $j \in \{1, \dots, n\}$ we have*

$$\mathbf{T}^{H_0,\dots,H_{j-1},H_j+tV_j,H_{j+1},\dots,H_n}_{f^{[n]}}(V_1, \dots, V_n) - \mathbf{T}^{H_0,\dots,H_n}_{f^{[n]}}(V_1, \dots, V_n) = t\mathbf{T}^{H_0,\dots,H_{j-1},H_j+tV_j,H_j,\dots,H_n}_{f^{[n+1]}}(V_1, \dots, V_j, V_j, \dots, V_n).$$

Proof. This is a special case of Theorem 50 in the appendix. □

4. Operator differentiation and Taylor series

4.1. First-order differentiation

In this subsection, we shall prove the following first-order differentiability result.

Theorem 17. *Let H be self-adjoint in (the separable Hilbert space) $\mathcal{H}$, let V be symmetric and relatively H-bounded, and let $u(x) := x - i$. Let $f \in C^1(\mathbb{R})$ be such that $f, (fu)' \in$*

$W_0(\mathbb{R})$. Then $t \mapsto f(H+tV)$ is Gateaux differentiable at $t=0$ in strong operator topology, and its Gateaux derivative equals

$$\frac{d}{dt} f(H+tV)\big|_{t=0} = \mathbf{T}^{H,H}_{f^{[1]}}(V) = T^{H,H}_{(fu)^{[1]}}(V(H-i)^{-1}) - f(H)V(H-i)^{-1}. \tag{10}$$

If, in addition, $V(H-i)^{-1} \in \mathcal{S}^\infty$, then $t \mapsto f(H+tV)$ is Gateaux differentiable in $t=0$ in operator norm topology, and its Gateaux derivative is given by (10).

The first step in the proof of Theorem 17 is the following adaptation of the Duhamel formula.

Lemma 18 *(Weighted Duhamel formula). Let H be self-adjoint in $\mathcal{H}$, and let V be symmetric and relatively H-bounded with H-bound < 1. For all $x \in \mathbb{R}$ and all $\psi \in \mathcal{H}$ we have*

$$e^{ix(H+V)}(H-i)^{-1}\psi - e^{ixH}(H-i)^{-1}\psi = ix \int_0^1 e^{isx(H+V)} V(H-i)^{-1} e^{i(1-s)xH}\psi \, ds,$$

where the integral on the right-hand side is a Bochner integral. Equivalently, for all $\varphi \in \operatorname{dom} H$ we have

$$e^{ix(H+V)}\varphi - e^{ixH}\varphi = ix \int_0^1 e^{isx(H+V)} V e^{i(1-s)xH}\varphi \, ds.$$

Proof. The proof looks similar to the proof of [4, Lemma 5.2], but needs some careful adjustments. Let $\psi \in \mathcal{H}$ be arbitrary. The function $G : \mathbb{R} \to \mathcal{H}$ defined by

$$G(s) := e^{isx(H+V)} e^{i(1-s)xH}(H-i)^{-1}\psi$$

is continuous by Stone's theorem. Moreover, for $\varphi := (H-i)^{-1}\psi$, we have $e^{i(1-s)xH}\varphi = (H-i)^{-1}e^{i(1-s)xH}\psi \in \operatorname{ran}(H-i)^{-1} = \operatorname{dom} H \subseteq \operatorname{dom} V$. Therefore, we obtain

$$\begin{aligned}
&\lim_{t\to 0}\left(\frac{G(s+t)-G(s)}{t}\right) \\
&= \lim_{t\to 0}\left(e^{i(s+t)x(H+V)} \frac{\left(e^{i(1-s-t)xH} - e^{i(1-s)xH}\right)}{t}\varphi \right. \\
&\qquad \left. + \frac{\left(e^{i(t+s)x(H+V)} - e^{isx(H+V)}\right)}{t}\left(e^{i(1-s)xH}\varphi\right)\right) \\
&= -ixe^{isx(H+V)} He^{i(1-s)xH}\varphi + ixe^{isx(H+V)}(H+V)e^{i(1-s)xH}\varphi \\
&= ixe^{isx(H+V)} V(H-i)^{-1} e^{i(1-s)xH}\psi,
\end{aligned} \tag{11}$$

by using Stone's theorem again and the fact that $e^{i(s+t)x(H+V)}$ is uniformly bounded by 1. (Indeed, to define this exponential we have already tacitly used the fact that $H+V$ is self-adjoint by Lemma 6(d).) By (11), the function $g : \mathbb{R} \to \mathcal{H}$ defined by

$$g(s) := ixe^{isx(H+V)}V(H-i)^{-1}e^{i(1-s)xH}\psi$$

is the derivative of G. As $V(H-i)^{-1}$ is bounded, it follows that g is continuous – without the right multiplication of $(H-i)^{-1}$, this argument would fail. The $\mathcal{H}$-valued fundamental theorem of calculus states

$$G(1) - G(0) = \int_0^1 g(s)\,ds,$$

where the right-hand side is a Bochner integral. By the definitions of G and g, we obtain the lemma. □

Lemma 19. *Let H be self-adjoint in $\mathcal{H}$, and let V be symmetric and relatively H-bounded with H-bound < 1. Let $f \in C^1(\mathbb{R})$ with $f, f' \in W_0(\mathbb{R})$, and let $\mu_{\hat{f}'}$ be the measure of which f' is the inverse Fourier transform. For all $\psi \in \mathcal{H}$ we have*

$$\begin{aligned}&f(H+V)(H-i)^{-1}\psi - f(H)(H-i)^{-1}\psi \\ &= \int_{\mathbb{R}} \int_0^1 e^{isx(H+V)}V(H-i)^{-1}e^{i(1-s)xH}\psi\,ds\,d\mu_{\hat{f}'}(x)\end{aligned}$$

Proof. The statement follows from Lemma 18, the dominated convergence theorem, and the fact that $ix\hat{f}(x) = \widehat{f'}(x)$ (when $\hat{f}, \widehat{f'}$ are functions, and similarly when they are measures). □

We may write the above formula in the more convenient MOI notation as follows.

Lemma 20. *Let H be self-adjoint in $\mathcal{H}$, and let V be symmetric and relatively H-bounded with H-bound < 1. For all $f \in C^1(\mathbb{R})$ with $f, f' \in W_0(\mathbb{R})$ we have*

$$\left(f(H+V) - f(H)\right)(H-i)^{-1} = T^{H+V,H}_{f^{[1]}}(V(H-i)^{-1}). \tag{12}$$

Proof. This is simply Lemma 19 combined with the definition of $T^{H+V,H}_{f^{[1]}}(V(H-i)^{-1})\psi$, cf. Corollary 12. □

Theorem 21. *Let H be self-adjoint in $\mathcal{H}$, and let V be symmetric and relatively H-bounded with H-bound < 1. Let $f \in \mathscr{W}_1(\mathbb{R})$, that is, let $f \in C^1(\mathbb{R})$ be such that $f, (fu)' \in W_0(\mathbb{R})$. We have*

$$f(H+V)-f(H)=T^{H+V,H}_{(fu)^{[1]}}(V(H-i)^{-1})-f(H+V)V(H-i)^{-1}.$$

Proof. From $f,(fu)'\in W_0(\mathbb{R})$ it follows that $f'\in W_0(\mathbb{R})$, and so we may apply Lemma 20. We now combine Lemma 20 with [27, Theorem 3.10], i.e., Theorem 47 below for $j=n=1$. We obtain

$$\begin{aligned}&(f(H+V)-f(H))(H-i)^{-1}\\&=T^{H+V,H}_{(fu)^{[1]}}(V(H-i)^{-2})-T^{H+V}_{f^{[0]}}()V(H-i)^{-2}\\&=\big(T^{H+V,H}_{(fu)^{[1]}}(V(H-i)^{-1})-f(H+V)V(H-i)^{-1}\big)(H-i)^{-1}.\end{aligned}$$

As $\operatorname{ran}(H-i)^{-1}=\operatorname{dom}H$, we obtain

$$(f(H+V)-f(H))\psi=\big(T^{H+V,H}_{(fu)^{[1]}}(V(H-i)^{-1})-f(H+V)V(H-i)^{-1}\big)\psi \tag{13}$$

for all $\psi\in\operatorname{dom}H$. As H is densely defined and the operators acting on ψ on both sides of (13) are bounded, the theorem follows. □

We now prove our main theorem of this section (existence of first-order Gateaux derivative).

Proof of Theorem 17. As tV is relatively bounded with H-bound <1 for all $t\in(-\frac{1}{a},\frac{1}{a})$ (see Lemma 6) we may apply Theorem 21 with tV in place of V. We obtain

$$\frac{f(H+tV)-f(H)}{t}=T^{H+tV,H}_{(fu)^{[1]}}(V(H-i)^{-1})-f(H+tV)V(H-i)^{-1}. \tag{14}$$

Firstly, we derive

$$\begin{aligned}\|f(H+tV)-f(H)\|&\le|t|\|T^{H+tV,H}_{(fu)^{[1]}}(V(H-i)^{-1})\|+|t|\|f(H+tV)V(H-i)^{-1}\|\\&\le|t|\left(\|\mu_1\|+\|f\|_\infty\right)\|V(H-i)^{-1}\|,\end{aligned}$$

which shows that

$$f(H+tV)\to f(H) \tag{15}$$

in norm as $t\to0$, where $(fu)'(x)=\int e^{ixy}d\mu_1(y)$. Moreover, we note for $\psi\in\mathcal{H}$ that

$$e^{isx(H+tV)}V(H-i)^{-1}e^{i(1-s)xH}\psi\to e^{isxH}V(H-i)^{-1}e^{i(1-s)xH}\psi,$$

for all $s\in[0,1]$ and all $x\in\mathbb{R}$. By the dominated convergence theorem, the above implies

$$T^{H+tV,H}_{(fu)^{[1]}}(V(H-i)^{-1})\psi\to T^{H,H}_{(fu)^{[1]}}(V(H-i)^{-1})\psi \tag{16}$$

for all $\psi \in \mathcal{H}$, i.e., convergence in the strong operator topology. If $V(H-i)^{-1}$ is compact, a similar argument shows that

$$T^{H+tV,H}_{(fu)^{[1]}}(V(H-i)^{-1}) \to T^{H,H}_{(fu)^{[1]}}(V(H-i)^{-1}) \tag{17}$$

in norm. Taking $t \to 0$ in the formula (14) and applying either (15) and (16) or (15) and (17) yields the theorem. □

4.2. Higher order differentiability

Theorem 22. *Let $n \in \mathbb{N}$ and $f \in \mathscr{W}_n(\mathbb{R})$. The following holds.*

(a) *For H self-adjoint in $\mathcal{H}$ and V symmetric and relatively H-bounded we have, in strong operator topology,*

$$\frac{1}{n!}\frac{d^n}{dt^n} f(H+tV)\big|_{t=0} = \mathbf{T}^{H,\dots,H}_{f^{[n]}}(V,\dots,V). \tag{18}$$

(b) *For H self-adjoint in $\mathcal{H}$ and V symmetric and relatively H-bounded with H-bound $a \in [0,\infty)$, for all $t_0 \in (-\frac{1}{a}, \frac{1}{a})$ we have, in strong operator topology,*

$$\frac{1}{n!}\frac{d^n}{dt^n} f(H+tV)\big|_{t=t_0} = \mathbf{T}^{H+t_0V,\dots,H+t_0V}_{f^{[n]}}(V,\dots,V).$$

Moreover, if we assume $V(H-i)^{-1} \in \mathcal{S}^\infty$, or we assume $f \in \mathscr{W}_{n+1}(\mathbb{R})$, then the above derivatives exist in operator norm topology.

Proof. From Lemma 6(d) and Lemma 6(e), it follows that (a) and (b) are equivalent. The rest of the proof consists of showing that (a) holds by induction to n. The base of the induction, that is, $n=1$, follows from Theorem 17.

Suppose, as an induction hypothesis, that (a) holds for a given $n \in \mathbb{N}$. It remains to show that (a) holds when n is replaced by $n+1$. Hence for each $f \in \mathscr{W}_{n+1}(\mathbb{R})$ we are to show the existence of, and compute, the strong operator (SOT) limit of the quotient

$$\begin{aligned}
&\frac{\frac{d^n}{ds^n} f(H+sV)\big|_{s=t} - \frac{d^n}{ds^n} f(H+sV)\big|_{s=0}}{t} \\
&= \frac{n!}{t}\left(\mathbf{T}^{H+tV,\dots,H+tV}_{f^{[n]}}(V,\dots,V) - \mathbf{T}^{H,\dots,H}_{f^{[n]}}(V,\dots,V)\right) \\
&= n! \sum_{k=0}^{n} \mathbf{T}_{f^{[n+1]}}^{\overbrace{H+tV,\dots,H+tV}^{n-k+1 \text{ times}},\overbrace{H,\dots,H}^{k+1 \text{ times}}}(V,\dots,V),
\end{aligned} \tag{19}$$

where we have used (b) in the first step, and used a telescoping sum together with Theorem 16 in the second step. Next, we find the SOT-limit of the 0th summand in

(19), noting that the limit of the other summands can be found in a similar way. By Theorem 15, we have

$$\begin{aligned}
&\mathbf{T}^{H+tV,\ldots,H+tV,H}_{f^{[n+1]}}(V,\ldots,V)\\
=&\sum_{p=0}^{n+1}(-1)^{n+1-p}\\
&\quad\times\sum_{0<j_1<\cdots<j_p\le n+1} T^{H_0(t),H_{j_1}(t),\ldots,H_{j_p}(t)}_{(fu^p)^{[p]}}(\tilde V_{0,j_1}(t),\ldots,\tilde V_{j_{p-1},j_p}(t))\tilde V_{j_p,n+1}(t)\\
=&(-1)^{n+1}f(H+tV)\left(V(H+tV-i)^{-1}\right)^n\left(V(H-i)^{-1}\right) \qquad (20)\\
&+\sum_{p=1}^{n+1}(-1)^{n+1-p}\\
&\quad\times\sum_{0<j_1<\cdots<j_p\le n+1} T^{H_0(t),H_{j_1}(t),\ldots,H_{j_p}(t)}_{(fu^p)^{[p]}}(\tilde V_{0,j_1}(t),\ldots,\tilde V_{j_{p-1},j_p}(t))\tilde V_{j_p,n+1}(t)
\end{aligned}$$

where $H_0(t)=\cdots=H_n(t)=H+tV$, $H_{n+1}(t)=H$, and $\tilde V_{j,l}(t):=V(H_{j+1}(t)-i)^{-1}\cdots V(H_l(t)-i)^{-1}\in\mathcal{B}(\mathcal{H})$. By Corollary 12, we have

$$\begin{aligned}
&T^{H_0(t),H_{j_1}(t),\ldots,H_{j_p}(t)}_{(fu^p)^{[p]}}(\tilde V_{0,j_1}(t),\ldots,\tilde V_{j_{p-1},j_p}(t))\\
&=\int_{\mathbb{R}}\int_{\Delta_p} e^{ixs_0H_0(t)}\tilde V_{0,j_1}(t)\,e^{ixs_1H_{j_1}(t)}\tilde V_{j_1,j_2}(t)\cdots\tilde V_{j_{p-1},j_p}(t)e^{ixs_pH_{J_p}(t)}\,ds\,d\mu_p(x),
\end{aligned}$$

where the measure $\mu_p=\widehat{(fu^p)^{(p)}}$ is the distributional Fourier transform of $(fu^p)^{(p)}\in C_b(\mathbb{R})\subseteq\mathcal{S}'(\mathbb{R})$. Next we note the following facts:

- By Lemma 6(e), $\|V(H+tV-i)^{-1}\|\le 2(a+b)$ for all $t\in[-\frac{1}{2a},\frac{1}{2a}]$.
- By the second resolvent identity (Lemma 7), for each $z\in\mathbb{C}$ with $Im\ z\neq 0$, $t\mapsto(H+tV-z)^{-1}$, $t\mapsto V(H+tV-z)^{-1}$ are continuous on $[-\frac{1}{2a},\frac{1}{2a}]$ in operator norm, and

$$\lim_{t\to 0}(H+tV-z)^{-1}=(H-z)^{-1}\quad\text{and}\quad\lim_{t\to 0}V(H+tV-z)^{-1}=V(H-z)^{-1}.$$

- For each fixed $x,s\in\mathbb{R}$, by [39, Theorem VIII.20], $t\mapsto e^{ixs(H+tV)}$, $t\mapsto f(H+tV)$ are both continuous on $[-\frac{1}{2a},\frac{1}{2a}]$ in the strong operator topology, and

$$SOT-\lim_{t\to 0}e^{is(H+tV)}=e^{isH}\quad\text{and}\quad SOT-\lim_{t\to 0}f(H+tV)=f(H).$$

- $$SOT-\lim_{t\to 0}e^{ixs_0H_0(t)}\tilde V_{0,j_1}(t)\,e^{ixs_1H_{j_1}(t)}\tilde V_{j_1,j_2}(t)\cdots\tilde V_{j_{p-1},j_p}(t)e^{ixs_pH_{j_p}(t)}$$

$$= e^{ixs_0H}\tilde{V}_{0,j_1}(0)\, e^{ixs_1H}\tilde{V}_{j_1,j_2}(0)\cdots\tilde{V}_{j_{p-1},j_p}(0)e^{ixs_pH} \tag{21}$$

- By Lemma 6(e), $\|e^{ixs_0H_0(t)}\tilde{V}_{0,j_1}(t)\, e^{ixs_1H_{j_1}(t)}\tilde{V}_{j_1,j_2}(t)\cdots\tilde{V}_{j_{p-1},j_p}(t)e^{ixs_pH_{j_p}(t)}\| \leq (2(a+b))^{j_1+\ldots+j_p}$ for all $t\in[-\frac{1}{2a},\frac{1}{2a}]$.

In conclusion, from the above, along with [12, Corollary III.6.16], we conclude that

$$\begin{aligned} SOT - \lim_{t\to 0} f(H+tV)\left(V(H+tV-i)^{-1}\right)^n \left(V(H-i)^{-1}\right) \\ = f(H)\left(V(H-i)^{-1}\right)^{n+1}, \text{ and} \end{aligned} \tag{22}$$

$$\begin{aligned} SOT - \lim_{t\to 0} T^{H_0(t),H_{j_1}(t),\ldots,H_{j_p}(t)}_{(fu^p)^{[p]}}(\tilde{V}_{0,j_1}(t),\ldots,\tilde{V}_{j_{p-1},j_p}(t)) \\ = T^{H_0(0),H_{j_1}(0),\ldots,H_{j_p}(0)}_{(fu^p)^{[p]}}(\tilde{V}_{0,j_1}(0),\ldots,\tilde{V}_{j_{p-1},j_p}(0)). \end{aligned} \tag{23}$$

The above limits together with (20) imply that

$$SOT - \lim_{t\to 0}\mathbf{T}^{H+tV,\ldots,H+tV,H}_{f^{[n+1]}}(V,\ldots,V) = \mathbf{T}^{H,\ldots,H}_{f^{[n+1]}}(V,\ldots,V).$$

By similar computations, we conclude that

$$SOT - \lim_{t\to 0}\mathbf{T}_{f^{[n+1]}}^{\overbrace{H+tV,\ldots,H+tV}^{n-k+1\text{ times}},\overbrace{H,\ldots,H}^{k+1\text{ times}}}(V,\ldots,V) = \mathbf{T}^{H,\ldots,H}_{f^{[n+1]}}(V,\ldots,V)$$

for every $0\leq k\leq n$. Therefore, from (19), we conclude that

$$\frac{1}{(n+1)!}\frac{d^{n+1}}{dt^{n+1}}f(H+tV)\Big|_{t=0} = \mathbf{T}^{H,\ldots,H}_{f^{[n+1]}}(V,\ldots,V) \tag{24}$$

in the strong operator topology. If we assume that $V(H-i)^{-1}$ is compact, then noting that the limits in (21), (22), and (23) exist in operator norm, we conclude that (24) exists in operator norm.

Next we show that, for $f\in\mathscr{W}_{n+1}(\mathbb{R})$, (18) exists in operator norm. By the same arguments as in the start of the proof, (a) and (b) are equivalent in this case as well. We shall prove (a) by induction on n. The base case $n=0$ is trivial. We shall show that (18) holds when n is replaced by $n+1$. By using (19), introducing another telescoping sum, and applying Theorem 16 again, now using the fact that $f\in\mathscr{W}_{n+2}(\mathbb{R})$, we obtain

$$\begin{aligned} &\frac{\frac{d^n}{ds^n}f(H+sV)\big|_{s=t} - \frac{d^n}{ds^n}f(H+sV)\big|_{s=0}}{t} - (n+1)!\mathbf{T}^{H,\ldots,H}_{f^{[n+1]}}(V,\ldots,V) \\ &= n!\sum_{k=0}^{n}\sum_{l=0}^{n-k}\Bigg(\mathbf{T}_{f^{[n+1]}}^{\overbrace{H+tV,\ldots,H+tV}^{l+1\text{ times}},\overbrace{H,\ldots,H}^{n-l+1\text{ times}}}(V,\ldots,V) \end{aligned}$$

$$-\mathbf{T}_{f^{[n+1]}}^{\overbrace{H+tV,\ldots,H+tV}^{l \text{ times}},\overbrace{H,\ldots,H}^{n-l+2 \text{ times}}}(V,\ldots,V)\Bigg)$$

$$= tn!\sum_{l=0}^{n}(n+1-l)\mathbf{T}_{f^{[n+2]}}^{\overbrace{H+tV,\ldots,H+tV}^{l+1 \text{ times}},\overbrace{H,\ldots,H}^{n-l+2 \text{ times}}}(V,\ldots,V).$$

From the operator-norm bound of $\mathbf{T}_{f^{[n+1]}}^{H_0,\ldots,H_{n+1}}(V,\ldots,V)$ given by Theorem 15, we obtain the bound

$$\left\| \frac{\frac{d^n}{ds^n} f(H+sV)\big|_{s=t} - \frac{d^n}{ds^n} f(H+sV)\big|_{s=0}}{t} - (n+1)!\mathbf{T}_{f^{[n+1]}}^{H,\ldots,H}(V,\ldots,V) \right\|$$

$$\leq |t|(n+2)!\sum_{p=0}^{n+2}\binom{n+2}{p}\frac{1}{p!}\|\mu_p\| \max\left(\left\|V(H-i)^{-1}\right\|, \left\|V(H+tV-i)^{-1}\right\|\right)^{n+1}.$$

From the above facts, we have $\left\|V(H+tV-i)^{-1}\right\| \leq \frac{a+b}{1-a}$. Hence, as $t \to 0$, the quotient on the left-hand side of (19) converges in norm to $(n+1)!\mathbf{T}_{f^{[n+1]}}^{H,\ldots,H}(V,\ldots,V)$, which shows by induction that (a) holds for all n. This completes the proof of the theorem. $\square$

Remark 23. Multi-variable Gateaux derivatives of operator functions can consequently be expressed in terms of (generalised) MOIs as

$$D_H^n f[V_1,\ldots,V_n] \equiv \frac{d}{dt_1}\cdots\frac{d}{dt_n} f(H+\sum_{i=1}^{n} t_i V_i)\Big|_{t=0}$$
$$= \sum_{\substack{\text{permutations } \sigma \\ \text{of } 1,\ldots,n}} \mathbf{T}_{f^{[n]}}^{H,\ldots,H}(V_{\sigma(1)},\ldots,V_{\sigma(n)}),$$

and analytic and algebraic properties of multi-variable Gateaux derivatives can be derived from those of MOIs, cf. Theorem 48, Theorem 50, and [29, Equation (4.2)].

Theorem 24. *(Taylor series) Let H be self-adjoint (possibly unbounded) in $\mathcal{H}$ and let V be symmetric and relatively H-bounded with H-bound $a \in [0,1)$. Let $f \in \cap_{n=1}^{\infty}\mathscr{W}_n(\mathbb{R})$ satisfy $\|\mu_n\| \leq c_f C_f^n n!$ for constants c_f, C_f such that $(1+C_f)\|V(H-i)^{-1}\| < 1$, where $(fu^n)^{(n)}(x) = \int e^{ixy} d\mu_n(y)$. We then have the Taylor expansion*

$$f(H+V) = \sum_{n=0}^{\infty} \frac{1}{n!}\frac{d^n}{dt^n} f(H+tV)\big|_{t=0},$$

which converges absolutely in operator norm.

Proof. By Theorem 22, the Taylor remainder can be written as

$$\begin{aligned}R_{n,H,f}(V) :=& f(H+V) - \sum_{k=0}^{n-1} \frac{1}{k!}\frac{d^k}{dt^k} f(H+tV)\big|_{t=0}\\ =& f(H+V) - \sum_{k=0}^{n-1} \mathbf{T}^{H,\ldots,H}_{f^{[k]}}(V,\ldots,V).\end{aligned}$$

By induction and Theorem 16 it follows that

$$R_{n,H,f}(V) = \mathbf{T}^{H+V,H,\ldots,H}_{f^{[n]}}(V,\ldots,V).$$

By applying Theorem 15 (note that $H_0 = H+V$ does not appear in the product $\prod_{j=1}^n \|V(H_j - i)^{-1}\|$), we obtain

$$\|R_{n,H,f}(V)\| \le \sum_{p=0}^{n} \binom{n}{p} \frac{1}{p!} \|\mu_p\| \|V(H-i)^{-1}\|^n,$$

and $\|\mathbf{T}^{H,\ldots,H}_{f^{[n]}}(V,\ldots,V)\|$ satisfies the exact same bound. By applying our assumption $\|\mu_p\| \le c_f C_f^p p!$ and putting the binomial theorem in reverse, we obtain

$$\|R_{n,H,f}(V)\| \le \sum_{p=0}^{n} \binom{n}{p} c_f C_f^p \|V(H-i)^{-1}\|^n = c_f(1+C_f)^n \|V(H-i)^{-1}\|^n.$$

If $(1+C_f)\|V(H-i)^{-1}\| < 1$ then $\|R_{n,H,f}(V)\| \to 0$ as $n \to \infty$ and so

$$f(H+V) = \|\cdot\|\text{-}\lim_{n\to\infty} \sum_{k=0}^{n-1} \frac{1}{k!}\frac{d^k}{dt^k} f(H+tV)\big|_{t=0}.$$

By the same argument, we have the absolute norm-convergence

$$\begin{aligned}&\sum_{n=0}^{\infty} \left\| \frac{1}{n!}\frac{d^n}{dt^n} f(H+tV)\big|_{t=0} \right\|\\ &\le \sum_{n=0}^{\infty} c_f (1+C_f)^n \|V(H-i)^{-1}\|^n = \frac{c_f}{1-(1+C_f)\|V(H-i)^{-1}\|} < \infty,\end{aligned}$$

concluding the proof. □

Lemma 25. *For $n \in \mathbb{N}$ and $f \in \bigcap_{n=1}^{\infty} \mathscr{W}_n(\mathbb{R})$, define the measures $\mu_n := \widehat{(fu^n)^{(n)}}$ and $\nu_n := \widehat{(f^{(n)}u^n)}$, the distributional Fourier transforms of $(fu^n)^{(n)}$ and $(f^{(n)}u^n)$, respectively. Denote $\mathscr{W}_{\mathrm{Taylor}}(\mathbb{R}) := \{f \in \cap_{n=1}^{\infty} \mathscr{W}_n(\mathbb{R}) \ :\ \exists c_f, C_f \ge 0\ \forall n \in \mathbb{N} : \|\mu_n\| \le c_f C_f^n n!\}$*

for the class of functions to which Theorem 24 (the Taylor series) applies. Denote $\mathscr{W}_{\text{CertainlyTaylor}}(\mathbb{R}) := \{f \in \cap_{n=1}^{\infty} \mathscr{W}_n(\mathbb{R}) \ : \ \exists c_f, C_f \geq 0 \ \forall n \in \mathbb{N} : \|\nu_n\| \leq c_f C_f^n n!\}$. *The following holds.*

(a) $\mathscr{W}_{\text{CertainlyTaylor}}(\mathbb{R}) \subseteq \mathscr{W}_{\text{Taylor}}(\mathbb{R})$.
(b) *If* $f, g \in \mathscr{W}_{\text{CertainlyTaylor}}(\mathbb{R})$, *then* $fg \in \mathscr{W}_{\text{CertainlyTaylor}}(\mathbb{R})$.
(c) *All bounded rational functions are in* $\mathscr{W}_{\text{CertainlyTaylor}}(\mathbb{R})$.
(d) *We have* $f \in \mathscr{W}_{\text{CertainlyTaylor}}(\mathbb{R})$ *for* $f(x) := e^{i\xi x} e^{-cx^2}$, $c > 0$, $\xi \in \mathbb{R}$.

Proof. Throughout the proof, we use the notation $a(n) \prec b(n)$ if there exist $c, C \geq 0$ such that $a(n) \leq cC^n b(n)$ for all $n \in \mathbb{N}$.

Statements (a) and (b) are both a straightforward check that employs the Fourier convolution theorem.

For (c), we let $u_w(x) := x - w$ for some $w \in \mathbb{C}$ with $Im\ w \neq 0$. Then

$$(u_w^{-1})^{(n)} = (-1)^n n! u_w^{-n-1},$$

and

$$u_w^{-1} u = 1 + (w - i) u_w^{-1},$$

and these formulas together with the binomial theorem imply that

$$(u_w^{-1})^{(n)} u^n = (-1)^n n! \sum_{k=0}^{n} \binom{n}{k} (w - i)^k u_w^{-k-1}. \tag{25}$$

By [33, Lemma 7] we have

$$\|\widehat{u_w^{-k-1}}\|_1 \prec \|u_w^{-k-1}\|_2 + \|(u_w^{-k-1})'\|_2. \tag{26}$$

Moreover, for all $m \in \{1, \ldots, n+2\}$ we have

$$\|u_w^{-m}\|_2^2 \prec \int_{\mathbb{R}} \frac{1}{(1 + x^2)^m}\, dx \leq \int_{\mathbb{R}} \frac{1}{1 + x^2}\, dx \prec 1. \tag{27}$$

Combining (25), (26), and (27), we obtain

$$\|((u_w^{-1})^{(n)} u^n)^\wedge\|_1 \prec n!.$$

Hence, $u_w \in \mathscr{W}_{\text{CertainlyTaylor}}(\mathbb{R})$. Consequently, by (b),

$$u_{w_1}^{-1} \cdots u_{w_n}^{-1} \in \mathscr{W}_{\text{CertainlyTaylor}}(\mathbb{R})$$

for all $w_i \in \mathbb{C}$ with $Im\ w_i \neq 0$. Since every bounded rational function on $\mathbb{R}$ is a linear combination of such functions, (c) is proven.

We now prove (d). We set $c = 1$ and $\xi = 0$ for simplicity, noting that the general case is proved analogously. We shall use the fact that, for $m \in \{0, \dots, 2n\}$,

$$\|\widehat{x^m e^{-x^2}}\|_1 \prec \sqrt{m!} \tag{28}$$

(see, e.g., [29, proof of Proposition 8(v)]). Write $f(x) = e^{-x^2}$. We note that $u^n(x) = \sum_{l=0}^{n} \binom{n}{l} x^l (-i)^{n-l}$, and that from the well-known explicit expression for the Hermite polynomials it follows that

$$f^{(n)}(x) = n! \sum_{m=0}^{\lfloor \frac{n}{2} \rfloor} \frac{(-1)^{m+n}}{m!(n-2m)!} (2x)^{n-2m} e^{-x^2}.$$

So,

$$f^{(n)}(x) u^n(x) = n! \sum_{l=0}^{n} \binom{n}{l} \sum_{m=0}^{\lfloor \frac{n}{2} \rfloor} \frac{(-i)^{n-l}(-1)^{m+n}}{m!(n-2m)!} x^l (2x)^{n-2m} e^{-x^2}.$$

Combining the latter with (28) yields

$$\|\widehat{f^{(n)} u^n}\|_1 \prec n! \sum_{l=0}^{n} \binom{n}{l} \sum_{m=0}^{\lfloor \frac{n}{2} \rfloor} \frac{1}{m!(n-2m)!} \sqrt{(n+l-2m)!}. \tag{29}$$

Stirling's approximation gives $k! \prec k^k$ and $k^k \prec k!$ for $k \in \{0, \dots, 2n\}$. This allows us to estimate, for all $m, l \leq n$,

$$\begin{aligned} \frac{1}{m!(n-2m)!} \sqrt{(n+l-2m)!} &\leq \frac{\sqrt{(2n-2m)!}}{m!(n-2m)!} \\ &\prec \frac{(2n-2m)^{n-m}}{m^m (n-2m)!} \\ &\prec \frac{m!(n-m)!}{(2m)!(n-2m)!} \\ &= \frac{m!(n-m)!}{n!} \frac{n!}{(2m)!(n-2m)!} \\ &\leq \binom{n}{2m}. \end{aligned} \tag{30}$$

Using the fact that $\sum_{s=0}^{p} \binom{p}{s} = 2^p \prec 1$ for all $p \leq n$, from combining (29) with (30) we get

$$\|\widehat{f^{(n)}u^n}\|_1 \prec n!\sum_{l=0}^{n}\binom{n}{l}\sum_{m=0}^{\lfloor \frac{n}{2}\rfloor}\binom{n}{2m} \prec n!,$$

as desired. We conclude that $f \in \mathscr{W}_{\text{CertainlyTaylor}}(\mathbb{R})$. □

Due to the relatively strong assumptions required for the convergence of the Taylor series for the function $t \mapsto f(H+tV)$, it is often more appropriate to focus on the Taylor remainder instead. In the next section, we examine the spectral properties of the Taylor remainder, particularly in relation to trace formulas and spectral shift functions.

5. Spectral shift functions

The next definition introduces the function class that features in our main theorem. Although it looks technical at first, the class neatly shows the influences of the summability parameter n, and the order k of the spectral shift function, on the required decay and differentiability of the function f. Let $u(\lambda) = (\lambda - i), \lambda \in \mathbb{R}$. For $x, y \in \mathbb{R}$, let $x \vee y = \max\{x, y\}$.

Definition 26. Let $n, k \in \mathbb{N}$. Let $\mathfrak{Q}_n^k(\mathbb{R})$ denote the space of all functions $f \in C^k(\mathbb{R})$ such that

(a) $fu^{2n} \in C_b(\mathbb{R})$,
(b) $f^{(l)}u^{n+l+1} \in C_0(\mathbb{R})$, $1 \leq l \leq k$, and
(c) $\widehat{f^{(k)}u^{k\vee n}} \in L^1(\mathbb{R})$.

We note the following properties of $f \in \mathfrak{Q}_n^k(\mathbb{R})$.

Proposition 27. *Let $n, k \in \mathbb{N}$. Then, for each $f \in \mathfrak{Q}_n^k(\mathbb{R})$,*

(a) $\widehat{f^{(l)}u^s} \in L^1(\mathbb{R})$ *for $s, l \in \mathbb{Z}_{\geq 0}$ such that $s \leq n \vee l$ and $l \leq k$;*
(b) $\big((fu^s)^{(l)}\big)\hat{\ } \in L^1(\mathbb{R})$ *for $s, l \in \mathbb{Z}_{\geq 0}$ such that $s \leq n \vee l$ and $l \leq k$;*
(c) $\mathfrak{Q}_n^k(\mathbb{R}) \subset \mathscr{W}_k(\mathbb{R})$.

Proof. Item (a) follows from Definition 26, the convolution theorem of the Fourier transform, and the well-known fact that $\hat{g} \in L^1(\mathbb{R})$ for all $g \in C^1(\mathbb{R})$ with $g, g' \in L^2(\mathbb{R})$. Item (b) follows from (a) and the Leibniz rule. Item (c) is immediate. □

Let $\mathfrak{R}_n := \{(\cdot - z)^{-l} : Im(z) \neq 0, l \in \mathbb{N}, l \geq 2n+1\}$, and let $\mathcal{S}(\mathbb{R})$ denote the class of Schwartz functions on $\mathbb{R}$. Then it follows from the definition of $\mathfrak{Q}_n^k(\mathbb{R})$ that

$$C_c^{k+1}(\mathbb{R}) \subset \mathfrak{Q}_n^k(\mathbb{R}) \subset C_0(\mathbb{R}), \quad \mathcal{S}(\mathbb{R}) \subset \mathfrak{Q}_n^k(\mathbb{R}), \text{ and } \mathfrak{R}_n \subset \mathfrak{Q}_n^k(\mathbb{R}).$$

As one straightforwardly checks that $\mathfrak{Q}_n^k(\mathbb{R})$ is an algebra, arbitrary products of functions in $C_c^{n+1}(\mathbb{R}) \cup \mathcal{S}(\mathbb{R}) \cup \mathfrak{R}_n$ are in $\mathfrak{Q}_n^k(\mathbb{R})$ as well.

Remark 28. For all $n, k_1, k_2 \in \mathbb{N}$, Proposition 27(a) implies that

$$\mathfrak{Q}_n^{k_1}(\mathbb{R}) \subseteq \mathfrak{Q}_n^{k_2}(\mathbb{R}) \text{ whenever } k_2 \leq k_1.$$

For proof of the following Lemma, we refer to [28, Lemma 2.4].

Lemma 29. *Let $n, m \in \mathbb{N} \cup \{0\}$, and let μ be a (finite) complex Radon measure on $\mathbb{R}$. For every $\epsilon \in (0,1]$ and every $k \in \mathbb{N} \cup \{0\}$ there exists a complex Radon measure $\tilde{\mu}_{k,\epsilon}$ with*

$$\|\tilde{\mu}_{k,\epsilon}\| \leq \left\|u^{-1-\epsilon}\right\|_1 \|\mu\|$$

and

$$\int_{\mathbb{R}} g^{(n)} u^m \, d\mu = \int_{\mathbb{R}} g^{(n+k)} u^{m+k+\epsilon} d\tilde{\mu}_{k,\epsilon} \tag{31}$$

for all $g \in C^{n+k}(\mathbb{R})$ satisfying $g^{(n+l)} u^{m+l} \in C_0(\mathbb{R})$, $l = 0, \ldots, k-1$ and $g^{(n+k)} u^{m+k-1} \in L^1(\mathbb{R})$.

Throughout this section, we shall refer to the following hypothesis.

Hypothesis 30. Let $n \in \mathbb{N}$, and let $n \geq 2$. Let H be self-adjoint in $\mathcal{H}$, and let V be symmetric and relatively H-bounded with H-bound < 1, that is,

$$\|V\psi\| \leq a \|H\psi\| + b \|\psi\| \text{ for all } \psi \in \operatorname{dom} H,$$

for some $a \in [0,1)$ and $b \in [0,\infty)$, such that

$$V(H-i)^{-p} \in \mathcal{S}^{n/p}, \qquad p \in \{1, \ldots, n\}. \tag{32}$$

We firstly remark that a symmetric operator V satisfying (32) is automatically relatively H-bounded, but the specific numbers a and b play a central role in several results below. We secondly remark that Hypothesis 30 for (n, H, V) implies Hypothesis 30 for $(n+1, H, V)$ *et cetera*. For improved function classes for the case $n = 1$, see [27, Theorem 4.1].

5.1. Krein spectral shift functions

In this subsection, we will obtain the Krein trace formula (first-order spectral shift formula) and the associated spectral shift function under Hypothesis 30. The following two lemmas are essential to prove our main results in this subsection.

Lemma 31. *Assume Hypothesis 30. There exists a sequence* $\{V_k\}_{k\in\mathbb{N}}$ *of finite rank self-adjoint operators such that*

(a) $\|V_k(H-i)^{-1}\|, \|V_k(H+V_k-i)^{-1}\| \leq \frac{a+b}{1-a}$;
(b) $\|\cdot\|_{n/p} - \lim_{k\to\infty} V_k(H-i)^{-p} = V(H-i)^{-p}$ *for* $1 \leq p \leq n$;
(c) $\|V_k(H-i)^{-p}\|_{n/p} \leq \|V(H-i)^{-p}\|_{n/p}$ *for* $1 \leq p \leq n$.

Proof. Let $E_H(\cdot)$ be the spectral measure of H. Let $k \in \mathbb{N}$, and let $P_k = E_H((-k,k))$. Then the following statements are true.

- for each $\psi \in \mathcal{H}$, $P_k\psi \in \operatorname{dom} H$,
- $SOT - \lim_{k\to\infty} P_k = I$.

Note that

$$P_kVP_k((H-i)^{-n}P_k + P_k^{\perp}) = P_kVP_k(H-i)^{-n}P_k = P_kV(H-i)^{-n}P_k \in \mathcal{S}^1. \quad (33)$$

By functional calculus it follows that $((H-i)^{-n}P_k + P_k^{\perp})$ is boundedly invertible. Hence, from (33), we have

$$P_kVP_k = P_kV(H-i)^{-n}P_k((H-i)^{-n}P_k + P_k^{\perp})^{-1} \in \mathcal{S}^1. \quad (34)$$

For each fixed $k \in \mathbb{N}$, by the spectral theorem there exists a sequence $\{E^l_{P_kVP_k}\}_{l\in\mathbb{N}}$ of finite rank projections such that

$$E^l_{P_kVP_k}P_kVP_k = P_kVP_kE^l_{P_kVP_k}, \text{ and } \|\cdot\|_1 - \lim_{l\to\infty} E^l_{P_kVP_k}P_kVP_k = P_kVP_k.$$

Therefore, there exists a strictly increasing sequence of natural numbers $\{l_k\}_{k\in\mathbb{N}}$ such that

$$\left\|E^{l_k}_{P_kVP_k}P_kVP_k - P_kVP_k\right\|_1 < \tfrac{1}{k}.$$

Let $V_k = E^{l_k}_{P_kVP_k}P_kVP_k$. Then

(a) For each $\psi \in \mathcal{H}$, $\|V_k\psi\| = \left\|E^{l_k}_{P_kVP_k}P_kVP_k\psi\right\| \leq \|VP_k\psi\| \leq a\|H\psi\| + b\|\psi\|$. Therefore, by Lemma 6(a) and Lemma 6(e), $\|V_k(H-i)^{-1}\|, \|V_k(H+V_k-i)^{-1}\| \leq \frac{a+b}{1-a}$.
(b) We have

$$\begin{aligned}
&\|V_k(H-i)^{-p} - V(H-i)^{-p}\|_{n/p} \\
&\leq \|V_k(H-i)^{-p} - P_kVP_k(H-i)^{-p}\|_{n/p} + \|P_kV(H-i)^{-p}P_k - V(H-i)^{-p}\|_{n/p} \\
&\leq \tfrac{1}{k} + \|P_kV(H-i)^{-p}P_k - V(H-i)^{-p}\|_{n/p} \longrightarrow 0 \text{ as } k \to \infty.
\end{aligned}$$

(c) We have $\|V_k(H-i)^{-p}\|_{n/p} = \|E^{l_k}_{P_kVP_k} P_kV(H-i)^{-p}P_k\|_{n/p} \le \|V(H-i)^{-p}\|_{n/p}$.

This completes the proof. □

Convention: Let H be a self-adjoint operator in $\mathcal{H}$, and V be a symmetric and relatively H-bounded with H bound a such that $V(H-i)^{-l} \in \mathcal{S}^k$ for some l, k. Then it is easy to show that $(H-i)^{-l}V$ equals $\big(V(H+i)^{-l}\big)^*$ on $\operatorname{dom} V$. As $\operatorname{dom} V$ is dense in $\mathcal{H}$, the operator $(H-i)^{-l}V$ has a unique bounded extension on the whole of $\mathcal{H}$, and we still denote this extension by $(H-i)^{-l}V$. Also, $V(H-i)^{-l} \in \mathcal{S}^k$ implies $(H-i)^{-l}V \in \mathcal{S}^k$ with $\|(H-i)^{-l}V\|_k = \|V(H+i)^{-l}\|_k$.

Lemma 32. *Let n, H, V satisfy Hypothesis 30. Let $(R, W) \in \{(0, V), (0, V_k), (V_k, V - V_k), (V_k, V_l - V_k)\}$, where $\{V_k\}_{k\in\mathbb{N}}$ is given by Lemma 31. For $t \in [0, 1]$, we denote*

$$H^t := H + R + tW.$$

For $1 \le p \le n$, define

$$\alpha_{n,V,H} := \max_{1\le p\le n} \|V(H-i)^{-p}\|_{n/p}. \tag{35}$$

Then

(a) *$(H^t-i)^{-p}W, W(H^t-i)^{-p} \in \mathcal{S}^{n/p}$, and*
(b) *$\|(H^t-i)^{-p}W\|_{n/p} = \|W(H^t-i)^{-p}\|_{n/p} \le 2^p\, \frac{1+b}{1-a}\, \alpha_{n,W,H} \max_{\ell=0,\,p-1}\{\alpha^{\ell}_{n,V,H}\}$.*

Proof. As $V_k \in \mathcal{B}(\mathcal{H})$, and the H-bound of V is < 1, it follows that R, W are relatively H-bounded and H^t-bounded. The equality in (b) follows directly from $(H^t+i)^{-l}W = (W(H^t-i)^{-l})^*$ (see the above convention), as this operator equals $(H^t-i)^{-l}W$ up to a unitary.

We prove the remaining results using mathematical induction on p. Let $p = 1$. Let $V_t := H^t - H$. By the second resolvent identity Lemma 7, we have

$$W[(H^t-i)^{-1} - (H-i)^{-1}] = -W(H-i)^{-1}V_t(H^t-i)^{-1}.$$

Note that $V_t = R + tW$ is H-bounded with H-bound $\le a < 1$. Hence, by Lemma 6(e), we have $\|V_t(H^t-i)^{-1}\| \le \frac{a+b}{1-a}$. Therefore, the above identity implies that

$$\begin{aligned}\|W(H^t-i)^{-1}\|_n &\le (1 + \frac{a+b}{1-a})\|W(H-i)^{-1}\|_n \\ &= \frac{1+b}{1-a}\|W(H-i)^{-1}\|_n. \end{aligned} \tag{36}$$

Thus (a) and (b) are true for $p = 1$.

Suppose (a) and (b) are true for $p = 1, 2, \ldots, m$ for some $m \in \{1, \ldots, n-1\}$. We will prove that (a) and (b) also hold for $p = m+1$. Indeed, a telescopic sum together with repeated applications of Lemma 7 yields

$$\begin{aligned}
&W[(H^t - i)^{-(m+1)} - (H - i)^{-(m+1)}] \\
&= W \sum_{l=0}^{m} \big((H^t - i)^{-1}\big)^l \big((H^t - i)^{-1} - (H - i)^{-1}\big)\big((H - i)^{-1}\big)^{m-l} \\
&= -\sum_{l=0}^{m} W(H^t - i)^{-(l+1)} V_t (H - i)^{-(m+1-l)}.
\end{aligned}$$

Therefore, using Hölder's inequality from the above identity we conclude

$$\begin{aligned}
&\|W(H^t - i)^{-(m+1)}\|_{n/(m+1)} \\
&\le \|W(H - i)^{-(m+1)}\|_{n/(m+1)} + \|W(H^t - i)^{-1}\|_n \, \|V(H - i)^{-m}\|_{n/m} \\
&\qquad + \sum_{l=1}^{m} \|W(H^t - i)^{-l}\|_{n/l} \, \|V(H - i)^{-(m+1-l)}\|_{n/(m+1-l)}. \qquad (37)
\end{aligned}$$

Let us write $C_p = \frac{1+b}{1-a} \alpha_{n,W,H} \max_{\ell=0,\,p-1} \{\alpha^l_{n,V,H}\}$, and consider the three terms on the right-hand side of (37). The first term is bounded by $\alpha_{n,W,H} \le C_{m+1}$, and thanks to (36) the second term is also bounded by C_{m+1}. By induction hypothesis, the third term is bounded by $\sum_{l=1}^{m} 2^l C_l \|V(H - i)^{-(m+1-l)}\|_{n/(m+1-l)} \le \sum_{l=1}^{m} 2^l C_{m+1}$. In total, we obtain

$$\|W(H^t - i)^{-(m+1)}\|_{n/(m+1)} \le 2^{m+1} C_{m+1},$$

proving the induction step. The lemma follows. □

Next, we recall known norm estimates of the classical MOI. The following estimate is a consequence of [43, Theorem 4.4.7 and Remark 4.4.2], first proven for $\tilde{H} = H$ in [34, Theorem 5.3 and Remark 5.4].

Theorem 33. *Let $k \in \mathbb{N}$ and let $\alpha, \alpha_1, \ldots, \alpha_k \in (1, \infty)$ satisfy $\frac{1}{\alpha_1} + \cdots + \frac{1}{\alpha_k} = \frac{1}{\alpha}$. Let $H, \tilde{H}$ be self-adjoint operators in $\mathcal{H}$. Assume that $V_m \in \mathcal{S}^{\alpha_m}$, $1 \le m \le k$. Then there exists $c_{\alpha,k} > 0$ such that*

$$\|T^{\tilde{H},H,\ldots,H}_{f^{[k]}}(V_1, V_2, \ldots, V_k)\|_\alpha \le c_{\alpha,k} \, \|f^{(k)}\|_\infty \prod_{1 \le m \le k} \|V_m\|_{\alpha_m} \qquad (38)$$

for every $f \in C^k_b(\mathbb{R})$ such that $\widehat{f^{(k)}} \in L^1(\mathbb{R})$.

The following theorem gives a key estimate to establish Krein's trace formula under Hypothesis 30.

Theorem 34. *Let n, H, V satisfy Hypothesis 30. Let $(R, W) \in \{(0, V), (V_l, V-V_l), (V_l, V_k-V_l)\}$, where $\{V_k\}_{k\in\mathbb{N}}$ is given by Lemma 31. Let $t \in [0,1]$, and denote $H^t = H+R+tW$. Then for each $f \in \mathfrak{Q}_n^1(\mathbb{R})$, we have*

$$\mathbf{T}_{f^{[1]}}^{H^t,H^t}(W) = T_{(fu^n)^{[1]}}^{H^t,H^t}(W(H^t-i)^{-n}) - \sum_{k=0}^{n-1}(fu^k)(H^t)W(H^t-i)^{-(k+1)} \in \mathcal{S}^1, \tag{39}$$

and each of the above $n+1$ summands is $\mathcal{S}^1$-continuous in t. Moreover,

$$\left|\mathrm{Tr}\left(T_{(fu^n)^{[1]}}^{H^t,H^t}(W(H^t-i)^{-n})\right)\right| \le \|(fu^n)^{(1)}\|_\infty \|W(H^t-i)^{-n}\|_1, \tag{40}$$

$$\left|\mathrm{Tr}\left(\sum_{k=0}^{n-1}(fu^k)(H^t)W(H^t-i)^{-(k+1)}\right)\right| \le n\|fu^{n-1}\|_\infty \|W(H^t-i)^{-n}\|_1. \tag{41}$$

Proof. Let $f \in \mathfrak{Q}_n^1(\mathbb{R})$. Then by repeated applications of Proposition 27, Theorem 14 and Lemma 10, we get

$$\begin{aligned}\mathbf{T}_{f^{[1]}}^{H^t,H^t}(W) =& T_{(fu)^{[1]}}^{H^t,H^t}(W(H^t-i)^{-1}) - f(H^t)W(H^t-i)^{-1}\\ =& T_{(fu^2)^{[1]}}^{H^t,H^t}(W(H^t-i)^{-2}) - (fu)(H^t)W(H^t-i)^{-2} - f(H^t)W(H^t-i)^{-1}\\ =& T_{(fu^n)^{[1]}}^{H^t,H^t}(W(H^t-i)^{-n}) - \sum_{k=0}^{n-1}(fu^k)(H^t)W(H^t-i)^{-(k+1)}.\end{aligned} \tag{42}$$

As Proposition 27 implies $\widehat{(fu^n)^{(1)}} \in L^1(\mathbb{R})$, Corollary 12 (namely, (8)), in particular means that $T_{(fu^n)^{(1)}}^{H^t,H^t}$ maps $\mathcal{S}^1$ to $\mathcal{S}^1$. Applying Lemma 32 therefore yields

$$T_{(fu^n)^{[1]}}^{H^t,H^t}(W(H^t-i)^{-n}) \in \mathcal{S}^1. \tag{43}$$

Since $t \mapsto (H^t-i)^{-1}$ is strongly continuous, it follows (see [37, Theorem VIII.20]) that $t \mapsto e^{isH^t}$ is strongly continuous. Hence, Corollary 12 and Lemma 32 also yield $\mathcal{S}^1$-continuity of the above operator in t.

Since $fu^{2n} \in C_b(\mathbb{R})$ by Definition 26(a), for each $0 \le k \le n-1$, by Lemma 32 we have

$$(fu^k)(H^t)W(H^t-i)^{-(k+1)} = (fu^{k+n})(H^t)(H^t-i)^{-n}W(H^t-i)^{-(k+1)} \in \mathcal{S}^1. \tag{44}$$

Thus, the identity (42) and the properties (43) and (44) together establish (39). The $\mathcal{S}^1$-continuity of (44) in t follows from Lemma 32 and strong continuity of $t \mapsto (fu^{k+n})(H^t)$, where the latter fact follows (see [37, Theorem VIII.20]) from the inclusion $fu^{k+n} \in C_b(\mathbb{R})$ and the strong continuity of $t \mapsto (H^t - i)^{-1}$.

By a standard DOI property of the general form "$\mathrm{Tr}(T^{D,D}_{g^{[1]}}(A)) = \mathrm{Tr}(g'(D)A)$", which in this case can be derived from Corollary 12, we have

$$\mathrm{Tr}\left(T^{H^t,H^t}_{(fu^n)^{[1]}}(W(H^t-i)^{-n})\right) = \mathrm{Tr}\left((fu^n)^{(1)}(H^t)\,(W(H^t-i)^{-n})\right).$$

Hence, by utilizing Hölder's inequality, we derive the estimate (40).

By using (44) and the cyclicity of the trace we conclude

$$\begin{aligned}\mathrm{Tr}\left((fu^k)(H^t)W(H^t-i)^{-(k+1)}\right) &= \mathrm{Tr}\left((H^t-i)^{-(k+1)}(fu^k)(H^t)W\right)\\ &= \mathrm{Tr}\left((fu^{n-1})(H^t)(H^t-i)^{-n}W\right).\end{aligned} \tag{45}$$

Applying Hölder's inequality to the right-hand side of (45), combined with the invariance of $\|\cdot\|_1$ under adjoints, results in the estimate (41). This concludes the proof. □

We briefly recall the classical result that the first-order spectral shift function exists for perturbations of trace class. This result is due to M. G. Krein [23], see also [49, Theorem 8.3.3].

Theorem 35 *(Krein). Let H be a self-adjoint operator in $\mathcal{H}$, and let $V = V^* \in \mathcal{S}^1$. Then there exists an integrable function ξ such that for all $f \in C^1(\mathbb{R})$ satisfying $\widehat{f'} \in L^1(\mathbb{R})$ (slightly more generally, $\widehat{f'}$ is only assumed to be a finite complex measure) we have*

$$\mathrm{Tr}(f(H+V) - f(H)) = \int_{-\infty}^{\infty} \xi(\lambda) f'(\lambda)\,d\lambda.$$

The following is the main result of this subsection.

Theorem 36. *Let n, H, V satisfy Hypothesis 30. Then there exists a locally integrable function $\eta_{1,H,V} \in L^1\left(\mathbb{R}, \frac{d\lambda}{(1+|\lambda|)^{n+\epsilon}}\right)$ such that*

$$\int_{\mathbb{R}} \frac{|\eta_{1,H,V}(\lambda)|}{(1+|\lambda|)^{n+\epsilon}} d\lambda \le n\,2^n \left(2n+3+2(n+1)\epsilon^{-1}\right) \frac{1+b}{1-a} \max_{\ell=1,\,n} \{\alpha^{\ell}_{n,V,H}\} \tag{46}$$

for all $\epsilon \in (0,1]$, where $\alpha_{n,V,H}$ is given by (35), and, moreover,

$$\mathrm{Tr}\left(f(H+V) - f(H)\right) = \int_{\mathbb{R}} f'(\lambda)\eta_{1,H,V}(\lambda) d\lambda \tag{47}$$

for every $f \in \mathfrak{Q}^1_n(\mathbb{R})$. The locally integrable function $\eta_{1,H,V}$ is determined by (47) uniquely up to an additive constant.

Proof. Let $f \in \mathfrak{Q}_n^1(\mathbb{R})$. Let $H_t = H + tV, t \in [0,1]$. By the fundamental theorem of calculus and using Theorem 22 we get the (a priori pointwise) integral

$$f(H+V) - f(H) = \int_0^1 \mathbf{T}_{f^{[1]}}^{H_t,H_t}(V)\,dt. \tag{48}$$

We now apply Theorem 34 to the above. By (40), (41), Lemma 32, and $\mathcal{S}^1$-continuity of the trace we may take the trace of the integral of (39) and find

$$\operatorname{Tr}(f(H+V) - f(H)) \tag{49}$$

$$= \operatorname{Tr}\left(\int_0^1 T^{H_t,H_t}_{(fu^n)^{[1]}}(V(H_t - i)^{-n})\,dt\right) - \operatorname{Tr}\left(\int_0^1 \sum_{k=0}^{n-1}(fu^k)(H_t)V(H_t-i)^{-(k+1)}dt\right) \tag{50}$$

$$= \alpha_1\big((fu^n)^{(1)}\big) + \alpha_2\big(fu^{n-1}\big) \tag{51}$$

for certain linear functionals α_1, α_2 defined on suitable subspaces of $C_0(\mathbb{R})$, and all $f \in \mathfrak{Q}_n^1(\mathbb{R})$. The above integrands are $\mathcal{S}^1$-continuous by Theorem 34, which shows that the above expressions are well defined and we may interchange trace with integral everywhere.

From (40) and (41) it follows that α_1 and α_2 are continuous in the supremum norm, and hence we may extend α_1 and α_2 to continuous functionals on $C_0(\mathbb{R})$. By the Riesz–Markov representation theorem, there exist two complex Borel measures μ_1, μ_2 such that

$$\operatorname{Tr}\left(f(H+V) - f(H)\right) = \int_{\mathbb{R}} (fu^n)^{(1)}(\lambda)d\mu_1(\lambda) + \int_{\mathbb{R}} (fu^{n-1})(\lambda)d\mu_2(\lambda)$$

$$= \int_{\mathbb{R}} \Big(f^{(1)}(\lambda)u^n(\lambda) + nf(\lambda)u^{n-1}(\lambda)\Big)d\mu_1(\lambda) + \int_{\mathbb{R}} (fu^{n-1})(\lambda)d\mu_2(\lambda), \tag{52}$$

and with total variation bounded by (40), (41) and Lemma 32(b) as

$$\begin{aligned}\|\mu_1\|, \|\mu_2\| &\le n\|V(H_t - i)^{-n}\|_1 \\ &\le n\,2^n\,\frac{1+b}{1-a}\max_{\ell=1,\,n}\{\alpha^{\ell}_{n,V,H}\}.\end{aligned} \tag{53}$$

For $\epsilon \in (0,1]$, applying Lemma 29 to (52) ensures the existence of a measure ν_ϵ such that

$$\operatorname{Tr}\left(f(H+V) - f(H)\right) = \int_{\mathbb{R}} f^{(1)}(\lambda)\,d\nu_\epsilon(\lambda) \qquad (f \in \mathfrak{Q}_n^1(\mathbb{R})) \tag{54}$$

with

$$\int_{\mathbb{R}} |u^{-n-\epsilon}(\lambda)| d|\nu_\epsilon|(\lambda) \le \|\mu_1\| + \|u^{-1-\epsilon}\|_1 (n\|\mu_1\| + \|\mu_2\|).$$

As $\frac{1}{1+|\lambda|} \le |u(\lambda)^{-1}|$, this further implies that

$$\begin{aligned}\int_{\mathbb{R}} \frac{d|\nu_\epsilon|(\lambda)}{(1+|\lambda|)^{n+\epsilon}} &\le \|\mu_1\| + \|u^{-1-\epsilon}\|_1 (n\|\mu_1\| + \|\mu_2\|) \\ &\le n\, 2^n \left(2n+3+2(n+1)\epsilon^{-1}\right) \frac{1+b}{1-a} \max_{\ell=1,\,n} \{\alpha^\ell_{n,V,H}\},\end{aligned} \tag{55}$$

where we have estimated $\|u^{-1-\epsilon}\|_1 = 2\int_0^1 |u^{-1-\epsilon}| + 2\int_1^\infty |u^{-1-\epsilon}| \le 2 + 2\epsilon^{-1}$.

Next, we will demonstrate that the measure ν_ϵ in (54) is absolutely continuous with respect to the Lebesgue measure. Let $\{V_k\}_{k\in\mathbb{N}}$ be the sequence given in Lemma 31. Therefore, by Theorem 35, there exists a sequence of integrable functions $\{\eta_{k,1}\}_{k\in\mathbb{N}}$ on $\mathbb{R}$ such that, for all $f \in C_c^\infty(\mathbb{R})$,

$$\operatorname{Tr}\left(f(H+V_k) - f(H)\right) = \int_{\mathbb{R}} f^{(1)}(\lambda)\, \eta_{k,1}(\lambda)\, d\lambda. \tag{56}$$

If $V_{k,l} := V_k - V_l$, then from (56), subsequently applying the fundamental theorem of calculus for MOIs (see [27, sentence below (42)]), and Theorem 34, we gather

$$\begin{aligned}&\left|\int_{\mathbb{R}} f^{(1)}(\lambda)(\eta_{k,1} - \eta_{l,1})(\lambda)\, d\lambda\right| \\ =&\left|\operatorname{Tr}\left(f(H+V_k) - f(H+V_l)\right)\right| \\ =&\left|\int_0^1 \operatorname{Tr}\left(\mathbf{T}_{f^{[1]}}^{H+V_l+tV_{k,l},H+V_l+tV_{k,l}}(V_{k,l})\right) dt\right| \\ \le&\left(\|(fu^n)^{(1)}\|_\infty + n\|fu^{n-1}\|_\infty\right) \int_0^1 dt\, \|V_{k,l}(H+V_l+tV_{k,l}-i)^{-n}\|_1.\end{aligned} \tag{57}$$

Thanks to Lemma 32, from (57) we obtain

$$\begin{aligned}&\left|\int_{\mathbb{R}} f^{(1)}(\lambda)(\eta_{k,1} - \eta_{l,1})(\lambda)\, d\lambda\right| \\ \le&\left(\|(fu^n)^{(1)}\|_\infty + n\|fu^{n-1}\|_\infty\right) 2^n \frac{1+b}{1-a}\, \alpha_{n,V_{k,l},H} \max_{p=0,\,n-1} \{\alpha^p_{n,V,H}\}.\end{aligned} \tag{58}$$

Let $f \in C_c^\infty((-d,d))$ for some fixed $d > 0$. Then, by using the standard estimates $\|gu^k\|_\infty \leq \|g\|_\infty (1+d)^k$ (for $g \in C_c^\infty((-d,d))$ and $\|f\|_\infty \leq 2d\|f'\|_\infty$, from (58) we get

$$\left|\int_{\mathbb{R}} f^{(1)}(\lambda)(\eta_{k,1}-\eta_{l,1})(\lambda)\,d\lambda\right| \tag{59}$$
$$\leq (1+d+4nd)\,(1+d)^{n-1}\,\|f^{(1)}\|_\infty\, 2^n\,\frac{1+b}{1-a}\,\alpha_{n,V_{k,l},H}\max_{p=0,\,n-1}\{\alpha^p_{n,V,H}\}.$$

Therefore, subsequently using (59) and Lemma 31(b) implies that

$$\begin{aligned}\|\eta_{k,1}-\eta_{l,1}\|_{L^1((-a,a))} &= \sup_{\|f^{(1)}\|_\infty\leq 1}\left|\int_{\mathbb{R}} f^{(1)}(\lambda)(\eta_{k,1}-\eta_{l,1})(\lambda)\,d\lambda\right| \\ &\leq (1+d+4nd)\,(1+d)^{n-1}\,2^n\,\frac{1+b}{1-a}\,\alpha_{n,V_{k,l},H}\max_{p=0,\,n-1}\{\alpha^p_{n,V,H}\} \\ &\longrightarrow 0 \text{ as } k,l\to\infty.\end{aligned}$$

Thus $\{\eta_{k,1}\}_{k\in\mathbb{N}}$ is a Cauchy sequence in $L^1_{loc}(\mathbb{R})$; we let η_1 be its $L^1_{loc}(\mathbb{R})$-limit. By a calculation completely analogous to (57)-(58), we conclude for $f \in C_c^\infty(\mathbb{R})$ that

$$\begin{aligned}\mathrm{Tr}\,(f(H+V)-f(H)) &= \lim_{k\to\infty}\mathrm{Tr}\,(f(H+V_k)-f(H)) \\ &= \lim_{k\to\infty}\int_{\mathbb{R}} f^{(1)}(\lambda)\,\eta_{k,1}(\lambda)\,d\lambda \\ &= \int_{\mathbb{R}} f^{(1)}(\lambda)\,\eta_1(\lambda)\,d\lambda.\end{aligned} \tag{60}$$

Now combining (54) and (60) we have the following equality

$$\int_{\mathbb{R}} f^{(1)}(\lambda)\,d\nu_\epsilon(\lambda) = \int_{\mathbb{R}} f^{(1)}(\lambda)\,\eta_1(\lambda)\,d\lambda \quad \text{for all} \quad f\in C_c^\infty(\mathbb{R}). \tag{61}$$

Let $d\mu(\lambda) = \eta_1(\lambda) - d\nu_\epsilon(\lambda)$. Then, it follows from (61) that

$$\int_a^b f^{(1)}(\lambda)d\mu(\lambda) = 0 \quad \text{for all } f \in C_c^\infty(\mathbb{R}). \tag{62}$$

Now consider the distribution T_μ defined by

$$T_\mu(\phi) := \int_a^b \phi\,d\mu(\lambda)$$

for every $\phi \in C_c^\infty(\mathbb{R})$. By (62) and the definition of the derivative of a distribution, $T_\mu^{(1)} = 0$. Hence by [3, Theorem 3.10 and Example 2.21], $d\mu(\lambda) = c\, d\lambda$ for some constant c. Consequently, $\eta_1 \in L^1_{loc}(\mathbb{R})$ satisfying (60) is unique up to an additive constant. In particular, we can assume $d\nu_\epsilon(\lambda) = \eta_1(\lambda)d\lambda$, and obtain

$$\int_{\mathbb{R}} \frac{|\eta_1(\lambda)|}{(1+|\lambda|)^{n+\epsilon}} d\lambda = \int_{\mathbb{R}} \frac{d|\nu_\epsilon|(\lambda)}{(1+|\lambda|)^{n+\epsilon}}.$$

By setting $\eta_{1,H,V} = \eta_1$, the above equality together with (54)-(55) completes the proof. □

5.2. Higher order spectral shift functions

The aim of this section is to provide all higher order spectral shift functions corresponding to a pair of self adjoint operators (H, V) satisfying the Hypothesis 30.

The following lemma is essential to reach our goal.

Lemma 37. *Let n, H, V satisfy Hypothesis 30. Write $\tilde{V} = V(H-i)^{-1}$. Then for $1 \le k \le n-1$, and $f \in \mathfrak{Q}_n^k(\mathbb{R})$,*

$$\begin{aligned} &\mathbf{T}_{f^{[k]}}^{H,\dots,H}(V,\dots,V) \qquad (63) \\ &= \sum_{l=0}^{k} \sum_{\substack{j_1+\dots+j_{l+1}=k \\ j_1,\dots,j_l \ge 1, j_{l+1} \ge 0}} \sum_{r=0}^{\min(n-k,l)} (-1)^{k-l+r} \sum_{\substack{p_0 \ge 0, p_1,\dots,p_r \ge 1 \\ p_0+\dots+p_r = n-k}} T_{(fu^{n-k+l-r})^{[l-r]}}^{H,\dots,H}(\tilde{V}^{j_1},\dots,\tilde{V}^{j_{l-r}}) \\ &\times (H-i)^{-p_0} \tilde{V}^{j_{l-r+1}} \cdots (H-i)^{-p_r} \tilde{V}^{j_{l+1}}. \end{aligned}$$

We recall that by standard convention, a product $B_1 \cdots B_m$ for $m < 1$ is 1, a list $(B_1, \dots, B_m)$ for $m < 1$ is the empty list $()$, and, by definition, $T_{g^{[0]}}^H() = g(H)$.

Proof. By Theorem 15, it follows that for any $k \ge 1$, and $f \in \mathfrak{Q}_n^k(\mathbb{R})$,

$$\mathbf{T}_{f^{[k]}}^{H,\dots,H}(V,\dots,V) = \sum_{l=0}^{k} \sum_{\substack{j_1+\dots+j_{l+1}=k \\ j_1,\dots,j_l \ge 1, j_{l+1} \ge 0}} (-1)^{k-l} T_{(fu^l)^{[l]}}^{H,\dots,H}\left(\tilde{V}^{j_1},\dots,\tilde{V}^{j_l}\right)\tilde{V}^{j_{l+1}}. \qquad (64)$$

We may now apply [29, Lemma 9] to each of the terms above, for $s = n-k$. Indeed, for all $l \in \{0,\dots,k\}$, from Proposition 27 it follows that fu^l is in the desired function class $\mathcal{W}^{n-k,l}$, in the notation of [29, Section 3]. The lemma follows immediately. □

The following theorem provides the existence of measures which are necessary to obtain the spectral shift functions of any order in the main theorem of this section.

Theorem 38. *Let n, H, V satisfy Hypothesis 30. Let $\epsilon \in (0,1]$. Then for each $k \in \mathbb{N}$,*

$$\mathbf{T}^{H,\ldots,H}_{f^{[k]}}(V,\ldots,V) \in \mathcal{S}^1,$$

and there exists a complex Borel measure $\mu_{k,\epsilon}$ such that

$$\operatorname{Tr}\left(\mathbf{T}^{H,\ldots,H}_{f^{[k]}}(V,\ldots,V)\right) = \int_{\mathbb{R}} f^{(k)}(\lambda) u^{k\vee n+\epsilon}(\lambda) d\mu_{k,\epsilon}(\lambda) \tag{65}$$

for every $f \in \mathfrak{Q}^k_n(\mathbb{R})$, with

$$\|\mu_{k,\epsilon}\| \leq c_{n,k,\epsilon}\, \alpha^k_{n,V,H}, \tag{66}$$

where $c_{n,k,\epsilon}$ is some positive constant, and $\alpha_{n,V,H}$ is given by (35).

Proof. For $1 \leq k < n$: By Lemma 37, we have the identity (63). Next we show that each term in the right hand side of (63) is a trace class operator and hence we can estimate the trace of those terms. Assuming the notations involved in (63), we note the following.

(i) Recalling that $T^H_{g^{[0]}}() = g(H)$, we notice that the summands corresponding to $r = l$ are of the form of (a minus sign times)

$$(fu^{n-k})(H)(H-i)^{-p_0}\tilde{V}^{j_1}\cdots(H-i)^{-p_l}\tilde{V}^{j_{l+1}}.$$

Employing a similar argument as given for (44), $fu^{2n} \in C_b(\mathbb{R})$ implies that

$$(fu^{n-k})(H)\tilde{V}^{j_1}\cdots(H-i)^{-p_l}\tilde{V}^{j_{l+1}} \in \mathcal{S}^1,$$

and using the cyclicity property of the trace along with Hölder's inequality for Schatten norms, this yields

$$\begin{aligned}
&\left|\operatorname{Tr}\left(\left(fu^{n-k}\right)(H)(H-i)^{-p_0}\tilde{V}^{j_1}(H-i)^{-p_1}\cdots\tilde{V}^{j_l}(H-i)^{-p_l}\tilde{V}^{j_{l+1}}\right)\right| \\
&= \left|\operatorname{Tr}\left(\left(fu^{n-k}\right)(H)\tilde{V}^{j_1}(H-i)^{-p_1}\cdots\tilde{V}^{j_l}(H-i)^{-p_l}\tilde{V}^{j_{l+1}}(H-i)^{-p_0}\right)\right| \\
&\leq \|fu^{n-k}\|_\infty\, \alpha^k_{n,V,H},
\end{aligned} \tag{67}$$

where $\alpha_{n,V,H}$ is given by (35).

(ii) For the rest of the terms in the summation of right hand side of (63): Now Proposition 27(b), Corollary 12, and Hölder's inequality for Schatten norms together imply

$$T^{H,\ldots,H}_{(fu^{n-k+l-r})^{[l-r]}}\left(\tilde{V}^{j_1},\ldots,\tilde{V}^{j_{l-r}}\right)(H-i)^{-p_1}\tilde{V}^{j_{l-r+1}}\cdots(H-i)^{-p_{r+1}}\tilde{V}^{j_{l+1}} \in \mathcal{S}^1.$$

If the product on the right of the multiple operator integral is nontrivial (either $r > 0$ or $j_{l+1} > 0$), then by applying Hölder's inequality for Schatten norms and using Theorem 33 we obtain

$$\left|\operatorname{Tr}\left(T^{H,\dots,H}_{(fu^{n-k+l-r})^{[l-r]}}\left(\tilde{V}^{j_1},\dots,\tilde{V}^{j_{l-r}}\right)(H-i)^{-p_1}\tilde{V}^{j_{l-r+1}}\cdots(H-i)^{-p_{r+1}}\tilde{V}^{j_{l+1}}\right)\right|$$
$$\leq d_{n,k}\,\|(fu^{n-k+l-r})^{(l-r)}\|_\infty\,\alpha^k_{n,V,H}, \tag{68}$$

where $d_{n,k}$ is a constant depending only on n and k.

The case where $r = 0$ and $j_{l+1} = 0$ takes a bit more care, because in the corresponding term $\operatorname{Tr}(T^{H,\dots,H}_{(fu^{n-k+l})^{[l]}}(\tilde{V}^{j_1},\dots,\tilde{V}^{j_l})(H-i)^{-(n-k)})$ the resolvent is not necessarily summable, and Theorem 33 is not applicable for $\alpha = 1$. Luckily, this case is similarly covered by [28, Lemma 2.9(i)] after commuting the resolvent inside the multiple operator integral.

Thus, (63) together with (i) and (ii) implies

$$\mathbf{T}^{H,\dots,H}_{f^{[k]}}(V,\dots,V) \in \mathcal{S}^1.$$

Having noted the remarks above, we apply the estimates (67) and (68), the Hahn-Banach theorem, and the Riesz–Markov representation theorem, and conclude that there exist complex Borel measures $\mu_{n,k,l,r}$, $0 \leq l \leq k$, $0 \leq r \leq \min\{n-k, l\}$ such that

$$\|\mu_{n,k,l,r}\| \leq \tilde{d}_{n,k}\,\alpha^k_{n,V,H}, \tag{69}$$

where $\tilde{d}_{n,k}$ is a constant depending only on n and k, and

$$\begin{aligned}
&\operatorname{Tr}\left(T^{H,\dots,H}_{f^{[k]}}(V,\dots,V)\right)\\
&=\sum_{l=0}^{k}\sum_{r=0}^{\min\{n-k,l\}}\int_{\mathbb{R}}\left(fu^{n-k+l-r}\right)^{(l-r)}(\lambda)\,d\mu_{n,k,l,r}(\lambda)\\
&=\sum_{l=0}^{k}\sum_{r=0}^{\min\{n-k,l\}}\sum_{s=0}^{l-r}\binom{l-r}{s}\int_{\mathbb{R}} f^{(s)}(\lambda)\,\left(u^{n-k+l-r}\right)^{(l-r-s)}(\lambda)\,d\mu_{n,k,l,r}(\lambda)\\
&=\sum_{\substack{0\leq l\leq k\\ 0\leq r\leq\min\{n-k,l\}\\ 0\leq s\leq l-r}}\binom{l-r}{s}\frac{(n-k+l-r)!}{(n-k+s)!}\int_{\mathbb{R}} f^{(s)}(\lambda)\,u^{n-k+s}(\lambda)\,d\mu_{n,k,l,r}(\lambda).
\end{aligned} \tag{70}$$

We note that $s \leq l \leq k$. Thanks to Lemma 29 and Equations (69) and (70), there exists a measure $\mu_{k,\epsilon}$ that satisfies (65) and (66), which completes the proof for $k < n$.

For $k \geq n$: Thanks to Equation (64), Theorem 33, and Hölder's inequality, we can argue similarly to the case $k < n$ and conclude the existence of a measure $\mu_{k,\epsilon}$ satisfying (65) and (66). This completes the proof. □

We proceed to present and demonstrate the central theorem of this section. In this theorem and its proof, the Taylor remainder is denoted

$$\mathcal{R}_{k,f,H}(V) := f(H+V) - \sum_{m=0}^{k-1} \frac{d^m}{dt^m} f(H+tV)\big|_{t=0}.$$

Theorem 39. *Let n, H, V satisfy Hypothesis 30. Then for each fixed $k \in \mathbb{N}$, there exists a locally integrable real-valued function $\eta_k := \eta_{k,H,V}$ such that*

$$\int_{\mathbb{R}} \frac{|\eta_k(\lambda)|}{(1+|\lambda|)^{n+k+\epsilon}} d\lambda \le C_{n,k,\epsilon} \frac{1+b}{1-a} \max_{\ell=1,\, k\vee n} \{\alpha_{n,V,H}^{\ell}\} \tag{71}$$

for all $\epsilon \in (0,1]$, where $C_{n,k,\epsilon}$ are some positive constants depending only on n, k, ϵ, and $\alpha_{n,V,H}$ is given by (35), and, moreover,

$$\operatorname{Tr}(\mathcal{R}_{k,f,H}(V)) = \int_{\mathbb{R}} f^{(k)}(\lambda)\eta_k(\lambda) d\lambda \tag{72}$$

for each $f \in \mathfrak{Q}_n^k(\mathbb{R})$. The locally integrable function η_k is determined by (72) uniquely up to a polynomial summand of degree at most $k-1$.

Proof. We prove (71) and (72) using the principle of mathematical induction on k. The base case, $k = 1$, of the induction follows from Theorem 36. Now we assume (71) and (72) are true for $k \in \{1, 2, \ldots, m\}$ for some $m \in \mathbb{N}$. Let $\epsilon \in (0,1]$. Let $f \in \mathfrak{Q}_n^{m+1}(\mathbb{R})$. Thanks to Theorem 22 and Theorem 38, there exists a finite complex Borel measure $\mu_{m,\epsilon}$ such that

$$\begin{aligned}\operatorname{Tr}(\mathcal{R}_{m+1,f,H}(V)) &= \operatorname{Tr}(\mathcal{R}_{m,f,H}(V)) - \operatorname{Tr}\left(\mathbf{T}_{f^{[m]}}^{H,\ldots,H}(V,\ldots,V)\right) \\ &= \int_{\mathbb{R}} f^{(m)}(\lambda)\eta_m(\lambda) d\lambda - \int_{\mathbb{R}} f^{(m)}(\lambda) u^{m\vee n+\epsilon}(\lambda) d\mu_{m,\epsilon}(\lambda).\end{aligned} \tag{73}$$

Next, by performing integration by parts on the right hand side of (73), we obtain

$$\operatorname{Tr}(\mathcal{R}_{m+1,f,H}(V)) = \int_{\mathbb{R}} f^{(m)}(\lambda)\, \eta_m(\lambda) d\lambda - \int_{\mathbb{R}} f^{(m)}(\lambda)\, u^{m\vee n+\epsilon}(\lambda) d\mu_{m,\epsilon}(\lambda)$$

$$= \int_{\mathbb{R}} f^{(m+1)}(\lambda) \left(-\int_0^{\lambda} \eta_m(t) dt \right) d\lambda + \int_{\mathbb{R}} f^{(m+1)}(\lambda)\, u^{m\vee n+\epsilon}(\lambda)\, \mu_{m,\epsilon}((-\infty,\lambda])\, d\lambda$$

$$- (m\vee n+\epsilon) \int_{\mathbb{R}} f^{(m+1)}(\lambda) \left(\int_0^{\lambda} u^{m\vee n+\epsilon-1}(t) \mu_{m,\epsilon}((-\infty,t])\, dt \right) d\lambda$$

$$= \int_{\mathbb{R}} f^{(m+1)}(\lambda)\eta_{m+1}(\lambda)d\lambda, \tag{74}$$

where

$$\begin{aligned} &\eta_{m+1}(\lambda) \\ =&u^{m\vee n+\epsilon}(\lambda)\mu_{m,\epsilon}((-\infty,\lambda]) \\ &-\int_0^\lambda \eta_m(t)dt - (m\vee n+\epsilon)\int_0^\lambda u^{m\vee n+\epsilon-1}(t)\mu_{m,\epsilon}\left((-\infty,t]\right)dt. \end{aligned} \tag{75}$$

Now, let us confirm that it follows from (66), (75), Theorem 36 and the induction hypothesis, that

$$\int_{\mathbb{R}} \frac{|\eta_{m+1}(\lambda)|}{(1+|\lambda|)^{n+m+1+\epsilon}}\,d\lambda \le \tilde{C}_{n,m+1,\epsilon}\,\frac{1+b}{1-a}\max_{\ell=1,\,m\vee n}\{\alpha^{\ell}_{n,V,H}\}, \tag{76}$$

for every $\epsilon\in(0,1]$, where $\tilde{C}_{n,m+1,\epsilon}$ is some positive constant. Indeed, the base case, $k=1$, of the induction follows from Theorem 36. Now, assume that the estimate (71) holds for $k=1,2,\dots,m$. It follows from (75) that

$$\begin{aligned} &\int_{\mathbb{R}} \frac{|\eta_{m+1}(\lambda)|}{(1+|\lambda|)^{n+m+1+\epsilon}}\,d\lambda \\ \le&\int_{\mathbb{R}} \frac{|u^{m\vee n+\epsilon}(\lambda)|\|\mu_{m,\epsilon}\|}{(1+|\lambda|)^{n+m+1+\epsilon}}\,d\lambda + \int_{\mathbb{R}}\int_{\mathbb{R}} \frac{1_{[0,\lambda]}(t)\,|\eta_m(t)|}{(1+|\lambda|)^{n+m+1+\epsilon}}\,dt\,d\lambda \\ &+(m\vee n+\epsilon)\int_{R} \frac{\int_0^\lambda |u^{m\vee n+\epsilon-1}(t)|\,\|\mu_{m,\epsilon}\|\,dt}{(1+|\lambda|)^{n+m+1+\epsilon}}\,d\lambda \\ \le&\int_{\mathbb{R}} \frac{\|\mu_{m,\epsilon}\|}{(1+|\lambda|)^{n+m+1-m\vee n}}\,d\lambda + \int_{\mathbb{R}} |\eta_m(t)|\left(\int_{\mathbb{R}} \frac{1_{[0,\lambda]}(t)}{(1+|\lambda|)^{n+m+1+\epsilon}}\,d\lambda\right)dt \\ &+(m\vee n+\epsilon)\int_{R} \frac{\|\mu_{m,\epsilon}\|}{(1+|\lambda|)^{n+m+1-m\vee n}}\,d\lambda. \end{aligned}$$

Now, by (66) and the induction hypothesis, the estimate (76) follows from the above. This completes the induction on k.

Since the left-hand side of (72) is real-valued whenever f is real-valued, we obtain that $Re\,\eta_k$ (instead of η_k) satisfies (72) for real-valued $f\in\mathfrak{Q}_n^k(\mathbb{R})$ and, consequently, for all $f\in\mathfrak{Q}_n^k(\mathbb{R})$. So we may assume η_k is real valued.

The uniqueness of η_k can be established in a similar manner as we did in Theorem 36. Indeed, suppose η_k and ξ_k satisfy (72), and let $\gamma_k = \eta_k - \xi_k$. Then from (72), we conclude

$$\int_{\mathbb{R}} f^{(k)}(\lambda)\gamma_k(\lambda)d\lambda = 0 \quad \text{for all } f \in C_c^\infty(\mathbb{R}). \tag{77}$$

Now consider the distribution T_{γ_k} defined by

$$T_{\gamma_k}(\phi) = \int_{\mathbb{R}} \phi(\lambda)\, \gamma_k(\lambda)d\lambda$$

for every $\phi \in C_c^\infty(\mathbb{R})$. By (77) and the definition of the derivative of a distribution, $T_{\gamma_k}^{(k)} = 0$. Hence by [3, Theorem 3.10 and Example 2.21], $\gamma_k(\lambda)d\lambda = f_k(\lambda)\, d\lambda$ for some polynomial f_k of degree at most $k-1$. Consequently, $\eta_k \in L^1_{loc}(\mathbb{R})$ satisfying (72) is unique up to a polynomial summand of degree at most $k-1$. Hence, we can assert that the estimates (72) hold true for all $\epsilon \in (0, 1]$. This completes the proof. □

Next, we provide the existence of n-th order spectral shift functions under a relaxed assumption compared to the above, which extends [27, Theorem 4.1] to the relatively bounded context.

Theorem 40. *Let $n \in \mathbb{N}$. Let H be a self-adjoint (unbounded) operator in $\mathcal{H}$, and let V be a symmetric and relatively H-bounded operator with H-bound $a \in [0, 1)$, that is,*

$$\|V\psi\| \le a\,\|H\psi\| + b\,\|\psi\| \ \textit{ for all } \psi \in \operatorname{dom} H, \ \textit{ for some } b \in [0, \infty),$$

such that $V(H-i)^{-1} \in \mathcal{S}^n$. Then, there exists $c_n > 0$ and a real-valued function η_n such that

$$\int_{\mathbb{R}} |\eta_n(x)|\, \frac{dx}{(1+|x|)^{n+\epsilon}} \le c_n\, (1+\epsilon^{-1})\, \frac{1+b}{1-a}\, \left\|V(H-i)^{-1}\right\|_n^n \quad \textit{for all } \epsilon > 0 \tag{78}$$

and

$$\operatorname{Tr}(\mathcal{R}_{n,f,H}(V)) = \int_{\mathbb{R}} f^{(n)}(x)\eta_n(x)\, dx \tag{79}$$

for every $f \in \mathfrak{W}_n$ (see [27, Definition 3.1]). The locally integrable function η_n is determined by (79) uniquely up to a polynomial summand of degree at most $n-1$.

Proof. The proof can be established along the same lines as the proof of [27, Theorem 4.1], by establishing analogous results to those of [27, Lemma 4.8, Lemma 4.9] in the relatively bounded setting. The latter can be achieved in a similar way as we did in Lemma 31 and Lemma 32, and Theorem 36. The replacement of the factor $(1+\|V\|)$ with $\frac{1+b}{1-a}$ is notable; these factors coincide if V is bounded. □

6. Applications

6.1. Applications: bounded perturbations

In this section we collect some known classes of examples of self-adjoint operators H and V satisfying our assumptions, namely $V \in \mathcal{B}(\mathcal{H})$ and

$$V(H-i)^{-p} \in \mathcal{S}^{n/p} \qquad (p = 1, \dots, n). \tag{80}$$

We merely scratch the surface of the collection of examples; more can be found in [27, 38,47,39], and references therein.

A result about Schatten class membership typically comes along with a bound on the Schatten norm, and by our main result these bounds imply estimates on the weighted integral norm of the spectral shift functions, for each specific situation. For brevity we omit these bounds, as they can be found in the respective cited references. Such bounds are called Cwikel estimates and Birman–Solomyak estimates, and form an active area of research [25,26].

6.1.1. Dirac and Laplace operators on Euclidean spaces

If, for suitable functions f, g on $\mathbb{R}^d$, the perturbation $V = M_f$ is the operator of multiplication by f, and moreover $(H-i)^{-p} = g(-i\nabla)$, where ∇ is the vector whose components are the operators $\{\partial_i\}_{i=1}^d$, then conditions for (80) to hold can be found in [8] and [39, Chapter 4]. As shown in the latter reference, such results typically require different proofs for $p \le n/2$ and $p > n/2$. Moreover, the spaces

$$\ell^p(L^q)(\mathbb{R}^d) := \left\{ f : \mathbb{R}^d \to \mathbb{C} \text{ measurable } : \sum_{k \in \mathbb{Z}^d} (\|f \restriction_{(0,1)^d+k} \|_{L^q(((0,1)^d+k))})^p < \infty \right\},$$

for $p \in [1, \infty)$ and $q \in [1, \infty]$, are frequently useful.

Two especially important examples of H are the Laplacian $H = \Delta = \sum_{k=1}^d \frac{\partial^2}{\partial x_k^2}$ in $L^2(\mathbb{R}^d)$ and the Dirac operator $H = D$, defined as

$$D := -i \sum_{k=1}^d e_k \otimes \frac{\partial}{\partial x_k}$$

in $\mathbb{C}^N \otimes L^2(\mathbb{R}^d)$, where $e_1, \dots, e_d \in M_N(\mathbb{C})$ are self-adjoint matrices satisfying $e_k e_l + e_l e_k = 2\delta_{k,l}$ for all $k, l \in \{1, \dots, d\}$. Here $N = 2^{d/2}$ if d is even and $N = 2^{(d+1)/2}$ if d is odd. The following result is proven in [42, Theorem III.4].

Theorem 41 *([42]). Let $m, d \in \mathbb{N}$ and $f \in \ell^1(L^2)(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ be real-valued, with associated multiplication operator M_f.*

(a) *If $n > d$, then*

$$(I \otimes M_f)(D - i)^{-p} \in \mathcal{S}^{n/p}, \qquad p = 1, \ldots, n.$$

(b) *If $n > \frac{d}{2}$, then*

$$M_f(\Delta - i)^{-p} \in \mathcal{S}^{n/p}, \qquad p = 1, \ldots, n.$$

6.1.2. The Hodge–Dirac operator on a Riemannian space

Part of the above result generalizes to suitable Riemannian manifolds, in the sense of the following theorem. For its proof we refer to [47, Equation (3.11)], which in that paper is proven in order to obtain [47, Theorem 3.4.1] by specializing to $p = d$.

Theorem 42 *([47]). Let (X, g) be a second countable d-dimensional complete smooth Riemannian manifold. Let $\Omega_c^k(X)$ be the space of smooth compactly supported differential k-forms, and $\mathcal{H}_k$ its completion with respect to the natural Hilbert space structure defined by g. Defined in the Hilbert space $\mathcal{H} := \oplus_{k=0}^d \mathcal{H}_k$, let D_g be the associated Hodge-Dirac operator. For $f \in C_c^\infty(X)$, let M_f denote the associated multiplication operator on $\mathcal{H}$. Then, for all $p \geq 1$ we have*

$$M_f(D_g - i)^{-p} \in \mathcal{S}^{d/p,\infty}.$$

Our main result thus becomes applicable by setting $n = d + 1$, and, independently of dimension, implies existence of spectral shift functions of all orders for Dirac operators on manifolds as in the above theorem.

In light of the above, it is reasonable to expect a generalization of Theorem 41 to exist for suitable Riemannian manifolds, but this is well beyond the scope of this text. A similar remark applies to matrix-valued differential operators and pseudodifferential operators.

6.1.3. Noncommutative geometry

Noncommutative geometry is a prime motivator for this paper, as it too is involved with proving results about geometrical objects – such as differential operators – without reference to their underlying space. The typical benefit for the noncommutative geometer is that the thus obtained results hold for more general objects which may not be geometrical, but may still be useful to describe physics.

A first application of the spectral shift function is to the theory of spectral flow [4], as used in index theory. Typically, one takes

$$H = D, \qquad V = u[D, u^*], \qquad \text{so that} \qquad H + V = uDu^*,$$

for a unitary u. More generally, perturbations in gauge theory take the form $V = \sum_{j=1}^n a_j[D, b_j]$, when a_j and b_j are elements of a 'smooth' algebra $\mathcal{A} \subseteq \mathcal{B}(\mathcal{H})$. Higher order spectral shift functions also provide analytical information on the Taylor remainders of the spectral action, which may be useful for the description of classical and quantum field theories [18,30].

The following result shows that our Hypothesis 30 holds for a wide class of nonunital spectral triples. It is a special case of [38, Proposition 10].

Theorem 43 *([38]). Let $(\mathcal{A}, \mathcal{H}, \mathcal{D})$ be a smooth local (d, ∞)-summable spectral triple in the sense of [38, Definition 7]. Then for all $a \in \mathcal{B}(\mathcal{H})$ satisfying $a\phi = \phi a = a$ for some $\phi \in \mathcal{A}_c$ we have*

$$a(\mathcal{D} - i)^{-p} \in \mathcal{S}^{(d+1)/p}, \qquad p = 1, \dots, d+1.$$

In particular cases one may expect strenghtenings of the above result. This is indeed the case for the Moyal plane $\mathbb{R}^d_\theta$, which is a prominent motivating example of a nonunital spectral triple. The result below follows from [25], as is written out explicitly below, for convenience of the reader.

Theorem 44 *([25]). Let $d \geq 2$ be even, $V \in W^{d,1}(\mathbb{R}^d_\theta)$, $h \in \mathbb{N}$, and set $n := \lfloor \frac{d}{h} \rfloor + 1$. For all $p \in \{1, \dots, n\}$, if we assume that $g \in \ell^{d/(hp),\infty}(L^\infty)(\mathbb{R}^d)$, then we have that $Vg(-i\nabla_\theta) \in \mathcal{S}^{n/p}$. In particular,*

$$V(D_\theta - i)^{-p} \in \mathcal{S}^{n/p} \qquad (p \in \{1, \dots, n\},\ n = d+1),$$

and

$$V(\Delta_\theta - i)^{-p} \in \mathcal{S}^{n/p} \qquad (p \in \{1, \dots, n\},\ n = d/2+1),$$

where D_θ and Δ_θ are the noncommutative Dirac and Laplace operators (see [25, p. 29]).

Proof. A combination of [25, Proposition 6.15(iii)], [25, Definition 6.14], and [25, Definition 6.7] yields $V \in W^{d,q}(\mathbb{R}^d_\theta)$ and thus $V \in L^q(\mathbb{R}^d_\theta)$ for all $q \geq 1$.

We define $n := \lfloor \frac{d}{h} \rfloor + 1$ and let $p \in \{1, \dots, n\}$, $h \in \mathbb{N}$, and $g \in \ell^{d/(hp),\infty}(L^\infty)(\mathbb{R}^d) \subseteq L^{d/(hp),\infty}(\mathbb{R}^d)$.

First suppose that $p \leq n/2$. Setting $q := d/(hp)$, a case distinction shows that $q \geq 1$. We find $g \in L^{q,\infty}(\mathbb{R}^d)$ and $V \in L^q(\mathbb{R}^d_\theta)$, hence [25, Lemma 2.3] implies that $V \otimes g \in \mathcal{L}_{q,\infty}(\mathcal{N})$, the noncommutative $L^{q,\infty}$-space of the von Neumann algebra $\mathcal{N} := L^\infty(\mathbb{R}^d_\theta) \otimes L^\infty(\mathbb{R}^d)$. In particular, since $n/p > d/(hp)$, we have $V \otimes g \in (\mathcal{L}_{n/p} \cap \mathcal{L}_\infty)(\mathcal{N})$. We note that $\frac{n}{p} \geq 2$ by assumption, so $L^{n/p} \cap L^\infty$ is an interpolation space for (L^2, L^∞). Therefore, [25, Theorem 7.2] gives

$$Vg(-i\nabla_\theta) \in \mathcal{L}_{n/p}(\mathcal{B}(L^2(\mathbb{R}^d))) = \mathcal{S}^{n/p}.$$

Now suppose that $p > n/2$. Set $q := \frac{n}{p} \in [1, 2)$ and note that $g \in \ell^q(L^\infty)(\mathbb{R}^d)$. We have $V \in W^{d,q}(\mathbb{R}^d_\theta)$ by Sobolev embedding, hence [25, Theorem 7.7] implies that

$$Vg(-i\nabla_\theta) \in \mathcal{L}_q(\mathcal{B}(L^2(\mathbb{R}^d))) = \mathcal{S}^{n/p},$$

completing the proof of the first statement.

To prove the second statement, one employs the functions g on $\mathbb{R}^d$ defined by

$$g(x) := (\gamma \cdot x - i)^{-p},$$
$$g(x) := (\|x\|^2 - i)^{-p},$$

where γ is the vector of Clifford matrices (see [25, Definition 6.17]). We indeed have $g \in \ell^{d/(hp),\infty}(L^\infty)(\mathbb{R}^d)$ for $h = 1$, $h = 2$, respectively. In the former case g is matrix-valued and this inclusion can be interpreted component-wise, the finite component $\mathbb{C}^{2^{\lfloor d/2 \rfloor}}$ of the Hilbert space factors through, and one indeed obtains $V(D_\theta - i)^{-p} \in \mathcal{S}^{n/p}(\mathbb{C}^{2^{\lfloor d/2 \rfloor}} \otimes L^2(\mathbb{R}^d))$ as well as $V(\Delta_\theta - i)^{-p} \in \mathcal{S}^{n/p}(L^2(\mathbb{R}^d))$. □

6.2. Applications: unbounded perturbations

Atomic Hamiltonians provide a rich class of examples in which the perturbation V is relatively bounded. The most basic example is the Hamiltonian of the hydrogen atom, i.e., the unbounded operator

$$H + V = -\frac{\hbar^2}{2m} \sum_i \frac{\partial^2}{\partial x_i^2} + V,$$

acting in $L^2(\mathbb{R}^d)$, where V is the Coulomb potential, namely, the multiplication operator

$$V\psi(x) = -\frac{e^2}{4\pi\epsilon_0} \frac{1}{\|x\|} \psi(x),$$

for physical constants $\hbar, m, e, \epsilon_0 \in \mathbb{R}$. A celebrated result of Kato ([20]) tells us that, indeed, V is relatively H-bounded. This result does not change if V is replaced by any other $L^2(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$-function, or if a larger number of possibly interacting particles are considered, either in H or V or both. In these atomic or molecular quantum systems, $a = 0$, and therefore (1) exists on $(-\infty, \infty)$, whereas a becomes nonzero in the 'relativistic case' where H is replaced with a Dirac operator D, and (1) exists on a bounded interval $(-\frac{1}{a}, \frac{1}{a})$. Clearly, the relatively bounded condition allows much more than these two classes of examples.

6.2.1. Finite-extent Coulomb potentials

In order to apply our results on the existence and regularity properties of the spectral shift functions (at all order), one needs to establish the n/p-summability of $V(H - i)^{-p}$.

It is known that the long-range behaviour of the Coulombic potential on $L^2(\mathbb{R}^3)$ obstructs Cwikel or Birman–Solomyak estimates. The following is a consequence of [39, Proposition 4.7]:

Lemma 45. *If $M_f(i+\Delta)^{-n} \in \mathcal{S}^1$ for some $n \in \mathbb{N}$, then $f \in \ell^1(L^2)(\mathbb{R}^d)$.*

As the next best thing (which suffices for many situations) one may consider spatially truncated (finite-extent) Coulomb potentials. By this we mean a compactly supported (or sufficiently decaying) function f which satisfies $f(x) = \frac{1}{\|x\|}$ for x in a compact region in $\mathbb{R}^d$. For such f, we have $f \in \ell^1(L^p)(\mathbb{R}^d)$ precisely when $p < d$. In particular, a finite-extent Coulomb potential on $\mathbb{R}^3$ is an example of an element in $\ell^1(L^2)(\mathbb{R}^3)$. In this case indeed, spectral shift functions of all orders exist.

Theorem 46. *For any $f \in \ell^1(L^2)(\mathbb{R}^3)$ and Δ the Laplacian on $\mathbb{R}^3$ we have*

$$M_f(i+\Delta)^{-p} \in \mathcal{S}^{4/p} \qquad (p = 1, 2, 3, 4).$$

Proof. Let $m \in \{2, 3, 4\}$. Define $g_m : \mathbb{R}^3 \to \mathbb{C}$ by

$$g_m(x) := (i - \|x\|^2)^{-m}.$$

Take $p_S := \frac{4}{m} \in [1, 2]$. Then $f \in \ell^1(L^2) \subseteq \ell^{p_S}(L^2)$ and $g_m \in \ell^{p_S}(L^2)$. By [39, Theorem 4.5], therefore

$$M_f(i+\Delta)^{-m} = M_f g_m(-i\nabla) \in \mathcal{S}^{4/m}.$$

We moreover note that $g_1 \in L^2(\mathbb{R}^3)$ and $f \in \ell^1(L^2)(\mathbb{R}^3) \subseteq L^2(\mathbb{R}^3)$. So by [39, Theorem 4.1], we obtain

$$M_f(i+\Delta)^{-1} = M_f g_1(-i\nabla) \in \mathcal{S}^2 \subseteq \mathcal{S}^4,$$

finishing the proof. □

It is clear from the above proof that there are various ways to improve Theorem 46; this is however beyond the scope of this text. For further results we refer to [50,49,21,37] and references therein.

Declaration of competing interest

On behalf of all authors, the corresponding author states that there is no conflict of interest.

Appendix A. Proofs of MOI identities

We give proofs of the identities claimed in §3.1. Throughout, whenever $\mathcal{J} \subseteq \{1, \ldots, n\}$ is such that $V_j \in \mathcal{B}(\mathcal{H})$ for $j \notin \mathcal{J}$, we use the notation

$$\mathbf{T}_{\phi,\mathcal{J}}(V_1,\dots,V_n) := \mathbf{T}_\phi(V_1,\dots,V_n) \tag{A.1}$$

to emphasise that V_j is possibly unbounded for $j \in \mathcal{J}$. In particular, $\mathbf{T}_{\phi,\emptyset} = T_\phi$.

A.1. Change of variables

In the case of bounded perturbations $V_1,\dots,V_n$, we recall the following result proved and used by Skripka and coathors in [9,27–29].

Theorem 47 *(change of variables). Let $H_0,\dots,H_n$ be self-adjoint and let $V_1,\dots,V_n \in \mathcal{B}(\mathcal{H})$ be bounded. For all $f \in C^n(\mathbb{R})$ with $f^{(n)}, f^{(n-1)}, (fu)^{(n)} \in W_0(\mathbb{R})$, we have for all $j \in \{1,\dots,n-1\}$,*

$$\begin{aligned} T^{H_0,\dots,H_n}_{f^{[n]}}(V_1,\dots,V_n) &= T^{H_0,\dots,H_n}_{(fu)^{[n]}}(V_1,\dots,V_{j-1},V_j(H_j-i)^{-1},V_{j+1},\dots,V_n) \\ &\quad - T^{H_0,\dots,H_{j-1},H_{j+1},\dots,H_n}_{f^{[n-1]}}(V_1,\dots,V_{j-1},V_j(H_j-i)^{-1}V_{j+1},V_{j+2},\dots,V_n). \end{aligned}$$

For the boundary case $j = n$ we similarly have

$$\begin{aligned} T^{H_0,\dots,H_n}_{f^{[n]}}(V_1,\dots,V_n) =& T^{H_0,\dots,H_n}_{(fu)^{[n]}}(V_1,\dots,V_{n-1},V_n(H_n-i)^{-1}) \\ & - T^{H_0,\dots,H_{n-1}}_{f^{[n-1]}}(V_1,\dots,V_{n-1})V_n(H_n-i)^{-1}, \end{aligned}$$

and for the boundary case $j = 0$ we have

$$\begin{aligned} T^{H_0,\dots,H_n}_{f^{[n]}}(V_1,\dots,V_n) =& T^{H_0,\dots,H_n}_{(fu)^{[n]}}((H_0-i)^{-1}V_1,V_2\dots,V_n) \\ & - (H_0-i)^{-1}V_1 T^{H_1,\dots,H_n}_{f^{[n-1]}}(V_2,\dots,V_n). \end{aligned}$$

We extend this theorem to relatively bounded arguments as follows. The following theorem is a rephrasing of Theorem 14 in the explicit notation (A.1).

Theorem 48 *(change of variables, relatively bounded). Let $H_0,\dots,H_n$ be self-adjoint. Let $\mathcal{J} \subseteq \{1,\dots,n\}$ be a subset so that V_k is bounded for each $k \in \{1,\dots,n\} \setminus \mathcal{J}$ and V_k is relatively H_k-bounded for each $k \in \mathcal{J}$. For each $f \in \mathscr{W}^n_{|\mathcal{J}|}(\mathbb{R})$ and each $j \in \{0,1,\dots,n\}$ (the boundary cases $j = 0$ and $j = n$ being understood as in Theorem 47) we have*

$$\begin{aligned} \mathbf{T}^{H_0,\dots,H_n}_{f^{[n]},\mathcal{J}}(V_1,\dots,V_n) &= \mathbf{T}^{H_0,\dots,H_n}_{(fu)^{[n]},\mathcal{J}\setminus\{j\}}(V_1,\dots,V_{j-1},V_j(H_j-i)^{-1},V_{j+1},\dots,V_n) \\ &\quad - \mathbf{T}^{H_0,\dots,H_{j-1},H_{j+1},\dots,H_n}_{f^{[n-1]},p_j^{-1}(\mathcal{J})}(V_1,\dots,V_{j-1},V_j(H_j-i)^{-1}V_{j+1},V_{j+2},\dots,V_n), \end{aligned}$$

where $p_j : \{1,\dots,n-1\} \to \{1,\dots,n\}$ is the order-preserving map whose range excludes j.

Proof. If $j \notin \mathcal{J}$, then the theorem follows directly from Definition 9 and Theorem 47, so we assume that $j \in \mathcal{J}$. For notational simplicity, we moreover assume that $j = 1$. We write $\alpha = (\alpha_1, \dots, \alpha_n) \in \{0,1\}^n$ where $\alpha_l = 1$ if and only if $l \in \mathcal{J}$. We also abbreviate $R_l := (H_l - i)^{-1}$. By definition,

$$\mathbf{T}^{H_0,\dots,H_n}_{f^{[n]},\mathcal{J}}(V_1,\dots,V_n) = T^{H_0,\dots,H_n}_{f^{[n]}u^\alpha}(V_1R_1^{\alpha_1},\dots,V_nR_n^{\alpha_n}). \tag{A.2}$$

We note that

$$f^{[n]}(\lambda_0,\dots,\lambda_n) = (fu)^{[n]}(\lambda_0,\dots,\lambda_n)u^{-1}(\lambda_1) - f^{[n-1]}(\lambda_0,\lambda_2,\dots,\lambda_n)u^{-1}(\lambda_1),$$

so also, for $\lambda = (\lambda_0,\dots,\lambda_n)$,

$$(f^{[n]}u^\alpha)(\lambda) = ((fu)^{[n]}u_1^{-1}u^\alpha)(\lambda) - f^{[n-1]}(\lambda_0,\lambda_2,\dots,\lambda_n)u^{-1}(\lambda_1)u^\alpha(\lambda),$$

and $u^{-1}(\lambda_1)u^\alpha(\lambda) = u^{\alpha_2}(\lambda_2)\cdots u^{\alpha_n}(\lambda_n)$. Therefore, denoting $\alpha' = (\alpha_2,\dots,\alpha_n)$, we have

$$(f^{[n]}u^\alpha)(\lambda) = ((fu)^{[n]}u^{\alpha-\delta_1})(\lambda) - (f^{[n-1]}u^{\alpha'})(\lambda_0,\lambda_2,\dots,\lambda_n), \tag{A.3}$$

where $\delta_1 = (1,0,\dots,0)$. Note that $|\mathcal{J}| = |\alpha|$. As $f \in \mathscr{W}^n_{|\alpha|}(\mathbb{R})$, we have $fu \in \mathscr{W}^n_{|\alpha-\delta_1|}(\mathbb{R})$ and $f \in \mathscr{W}^{n-1}_{|\alpha'|}(\mathbb{R})$ by Lemma 4(a). Hence, by (A.2), (A.3), and Theorem 13 we have

$$\begin{aligned}\mathbf{T}^{H_0,\dots,H_n}_{f^{[n]},\mathcal{J}}(V_1,\dots,V_n) =& T^{H_0,\dots,H_n}_{(fu)^{[n]}u^{\alpha-\delta_1}}(V_1R_1^{\alpha_1},V_2R_2^{\alpha_2},\dots,V_nR_n^{\alpha_n})\\ &- T^{H_0,H_2,\dots,H_n}_{f^{[n-1]}u^{\alpha'}}(V_1R_1^{\alpha_1}V_2R_2^{\alpha_2},V_3R_3^{\alpha_3},\dots,V_nR_n^{\alpha_n})\\ =&\mathbf{T}^{H_0,\dots,H_n}_{(fu)^{[n]},\mathcal{J}\setminus\{1\}}(V_1(H_1-i)^{-1},V_2,\dots,V_n)\\ &- \mathbf{T}^{H_0,H_2,\dots,H_n}_{f^{[n-1]},p_1^{-1}(\mathcal{J})}(V_1(H_1-i)^{-1}V_2,V_3,\dots,V_n),\end{aligned}$$

which completes the proof. □

A.2. Superscript difference

The following proposition is an extension of Theorem 21 to higher order, and an extension of [43, Theorem 4.3.14] to relatively bounded differences $A - B$, and is a step towards its generalization involving general multilinear symbols $\mathbf{T}^{H_0,\dots,H_n}_{f^{[n]},\mathcal{J}}$.

Proposition 49. *Let $n \in \mathbb{N}_{\geq 1}$ and $j \in \{1,\dots,n\}$. Let $H_0,\dots,H_n$ be self-adjoint, let $V_1,\dots,V_{n-1} \in \mathcal{B}(\mathcal{H})$, and let V_n be a relatively H_n-bounded operator. Let V be symmetric and relatively H_j-bounded with H_j-bound < 1 and suppose that V_j is relatively $H_j + V$-bounded (for instance, if V is a scalar multiple of V_j). Write $A = H_j + V$, $B = H_j$. For all $f \in \mathscr{W}^{n+1}_2(\mathbb{R})$ (i.e. $f \in C^{n+1}(\mathbb{R})$ such that $f^{(n-1)}, (fu)^{(n)}, (fu^2)^{(n+1)} \in W_0(\mathbb{R})$) we have*

$$\mathbf{T}^{H_0,\ldots,H_{j-1},A,H_{j+1},\ldots,H_n}_{f^{[n]},\{n\}}(V_1,\ldots,V_n) - \mathbf{T}^{H_0,\ldots,H_{j-1},B,H_{j+1},\ldots,H_n}_{f^{[n]},\{n\}}(V_1,\ldots,V_n)$$
$$= \mathbf{T}^{H_0,\ldots,H_{j-1},A,B,H_{j+1},\ldots,H_n}_{f^{[n+1]},\{j+1,p_{j+1}(n)\}}(V_1,\ldots,V_j,A-B,V_{j+1},\ldots,V_n),$$

where $p_{j+1} : \{1,\ldots,n\} \to \{1,\ldots,n+1\}$ *is the order-preserving map whose range excludes* $j+1$.

Proof. We prove the statement for $j = 1$ for notational simplicity; the proof for other values of j is completely analogous. Similarly we assume $n \geq 2$. We shall denote $\tilde{V}_n = V_n(H_n - i)^{-1}$. It follows from Definition 9 together with the fact that $f^{[n]}u^{(0,\ldots,0,1)} \in \mathfrak{BS}(\mathbb{R}^{n+1})$ that

$$\begin{aligned}\mathbf{T}^{H_0,A,H_2,\ldots,H_n}_{f^{[n]},\{n\}}(V_1,\ldots,V_n)(H_n-i)^{-1} &= T^{H_0,A,H_2,\ldots,H_n}_{f^{[n]}u^{(0,\ldots,0,1)}}(V_1,\ldots,\tilde{V}_n)(H_n-i)^{-1} \\ &= T^{H_0,A,H_2,\ldots,H_n}_{f^{[n]}u^{(0,\ldots,0,1)}}(V_1,\ldots,\tilde{V}_n(H_n-i)^{-1}) \\ &= \mathbf{T}^{H_0,A,H_2,\ldots,H_n}_{f^{[n]},\{n\}}(V_1,\ldots,\tilde{V}_n) \\ &= T^{H_0,A,H_2,\ldots,H_n}_{f^{[n]}}(V_1,\ldots,\tilde{V}_n), \end{aligned} \tag{A.4}$$

where the last equality follows from Lemma 10. Since $(fu)^{(n)} \in W_0(\mathbb{R})$, by Corollary 12, we have

$$\begin{aligned} &T^{H_0,A,H_2,\ldots,H_n}_{(fu)^{[n]}}(V_1(A-i)^{-1},V_2,\ldots,V_n) \\ &= \int_{\mathbb{R}}\int_{\Delta_n} e^{is_0xH_0}V_1(A-i)^{-1}e^{is_1xA}V_2e^{is_2xH_2}\cdots V_ne^{is_nxH_n}\,ds\,d\mu(x) \\ &= \int_{\mathbb{R}}\int_{\Delta_n} e^{is_0xH_0}V_1e^{is_1xA}(A-i)^{-1}V_2e^{is_2xH_2}\cdots V_ne^{is_nxH_n}\,ds\,d\mu(x) \\ &= T^{H_0,A,H_2,\ldots,H_n}_{(fu)^{[n]}}(V_1,(A-i)^{-1}V_2,\ldots,V_n), \end{aligned} \tag{A.5}$$

where $(fu)^{(n)}(x) = \int e^{ixy}d\mu(y)$.

Now by first using the identity (A.4), then using change-of-variables (Theorem 47), then using the identity (A.5), then using the second resolvent identity (Lemma 7), we obtain

$$\begin{aligned} &\Big(\mathbf{T}^{H_0,A,H_2,\ldots,H_n}_{f^{[n]},\{n\}}(V_1,\ldots,V_n) - \mathbf{T}^{H_0,B,H_2,\ldots,H_n}_{f^{[n]},\{n\}}(V_1,\ldots,V_n)\Big)(H_n-i)^{-1} \\ &= T^{H_0,A,H_2,\ldots,H_n}_{f^{[n]}}(V_1,\ldots,\tilde{V}_n) - T^{H_0,B,H_2,\ldots,H_n}_{f^{[n]}}(V_1,\ldots,\tilde{V}_n) \\ &= T^{H_0,A,H_2,\ldots,H_n}_{(fu)^{[n]}}(V_1,(A-i)^{-1}V_2,V_3,\ldots,\tilde{V}_n) \\ &\quad - T^{H_0,H_2,\ldots,H_n}_{f^{[n-1]}}(V_1(A-i)^{-1}V_2,V_3,\ldots,\tilde{V}_n) \\ &\quad - T^{H_0,B,H_2,\ldots,H_n}_{(fu)^{[n]}}(V_1,(B-i)^{-1}V_2,V_3,\ldots,\tilde{V}_n) \end{aligned}$$

$$
\begin{aligned}
&+ T^{H_0,H_2,\ldots,H_n}_{f^{[n-1]}}(V_1(B-i)^{-1}V_2, V_3, \ldots, \tilde{V}_n) \\
= &- T^{H_0,A,H_2,\ldots,H_n}_{(fu)^{[n]}}(V_1, (A-i)^{-1}(A-B)(B-i)^{-1}V_2, V_3, \ldots, \tilde{V}_n) \\
&+ T^{H_0,A,H_2,\ldots,H_n}_{(fu)^{[n]}}(V_1, (B-i)^{-1}V_2, V_3, \ldots, \tilde{V}_n) \\
&- T^{H_0,B,H_2,\ldots,H_n}_{(fu)^{[n]}}(V_1, (B-i)^{-1}V_2, V_3, \ldots, \tilde{V}_n) \\
&+ T^{H_0,H_2,\ldots,H_n}_{f^{[n-1]}}(V_1(A-i)^{-1}(A-B)(B-i)^{-1}V_2, V_3, \ldots, \tilde{V}_n). \qquad \text{(A.6)}
\end{aligned}
$$

The second and third term on the right-hand side can be combined as follows. Both multiple operator integrals have purely bounded arguments, so when applied to a vector $\psi \in \mathcal{H}$ they can be written as $\mathcal{H}$-valued integrals over a finite measure obtained from the Fourier transform of $(fu)^{(n)} \in W_0(\mathbb{R})$. Note that $(fu)^{(n+1)} \in W_0(\mathbb{R})$. Arguing as in the proof of [4, Eq. (5.6)], namely by first invoking Corollary 12, then applying the weighted Duhamel formula (Lemma 18), and finally using Fubini's theorem ([4, Lemma 3.8]), we obtain for $\psi \in \mathcal{H}$ that

$$
\begin{aligned}
&T^{H_0,A,H_2,\ldots,H_n}_{(fu)^{[n]}}(V_1, (B-i)^{-1}V_2, V_3, \ldots, \tilde{V}_n)\psi \\
&- T^{H_0,B,H_2,\ldots,H_n}_{(fu)^{[n]}}(V_1, (B-i)^{-1}V_2, V_3, \ldots, \tilde{V}_n)\psi \\
= &\int_{\mathbb{R}} \int_{\Delta_n} e^{is_0xH_0} V_1 \big(e^{is_1xA} - e^{is_1xB}\big)(B-i)^{-1} V_2 e^{is_2xH_2} \cdots V_n e^{is_nxH_n}\, \psi \, ds \, d\mu(x) \\
= i &\int_{\mathbb{R}} \int_{\Delta_n} e^{is_0xH_0} V_1 \Big(\int_0^{s_1} e^{itxA}(A-B) e^{i(s_1-t)xB}\, dt \Big) \\
&\times (B-i)^{-1} V_2 e^{is_2xH_2} \cdots V_n e^{is_nxH_n}\, \psi \, ds \, d\mu(x) \\
= i &\int_{\mathbb{R}} \int_{\Delta_n} \int_0^{s_1} e^{is_0xH_0} V_1 e^{itxA}(A-B) \\
&\times (B-i)^{-1} e^{i(s_1-t)xB} V_2 e^{is_2xH_2} \cdots V_n e^{is_nxH_n}\, \psi \, dt \; ds \, d\mu(x) \\
= &T^{H_0,A,B,H_2,\ldots,H_n}_{(fu)^{[n+1]}}(V_1, (A-B)(B-i)^{-1}, V_2, V_3, \ldots, \tilde{V}_n)\psi,
\end{aligned}
$$

where in the third equality, we use that $(B-i)^{-1}e^{i(s_1-t)xB} = e^{i(s_1-t)xB}(B-i)^{-1}$. Therefore,

$$
\begin{aligned}
&T^{H_0,A,H_2,\ldots,H_n}_{(fu)^{[n]}}(V_1, (B-i)^{-1}V_2, V_3, \ldots, \tilde{V}_n)\psi \\
&\quad - T^{H_0,B,H_2,\ldots,H_n}_{(fu)^{[n]}}(V_1, (B-i)^{-1}V_2, V_3, \ldots, \tilde{V}_n) \\
= &T^{H_0,A,B,H_2,\ldots,H_n}_{(fu)^{[n+1]}}(V_1, (A-B)(B-i)^{-1}, V_2, V_3, \ldots, \tilde{V}_n).
\end{aligned}
$$

Substituting this in (A.6), we find

$$
\begin{aligned}
X(H_n-i)^{-1} :=& \Big(\mathbf{T}^{H_0,A,H_2,\ldots,H_n}_{f^{[n]},\{n\}}(V_1,\ldots,V_n) - \mathbf{T}^{H_0,B,H_2,\ldots,H_n}_{f^{[n]},\{n\}}(V_1,\ldots,V_n)\Big)(H_n-i)^{-1} \\
=& -T^{H_0,A,H_2,\ldots,H_n}_{(fu)^{[n]}}(V_1,(A-i)^{-1}(A-B)(B-i)^{-1}V_2,V_3,\ldots,\tilde{V}_n) \\
&+ T^{H_0,A,B,H_2,\ldots,H_n}_{(fu)^{[n+1]}}(V_1,(A-B)(B-i)^{-1},V_2,V_3,\ldots,\tilde{V}_n) \\
&+ T^{H_0,H_2,\ldots,H_n}_{f^{[n-1]}}(V_1(A-i)^{-1}(A-B)(B-i)^{-1}V_2,V_3,\ldots,\tilde{V}_n) \\
=& -T^{H_0,A,H_2,\ldots,H_n}_{f^{[n]}}(V_1,(A-B)(B-i)^{-1}V_2,V_3,\ldots,\tilde{V}_n) \\
&+ T^{H_0,A,B,H_2,\ldots,H_n}_{(fu)^{[n+1]}}(V_1,(A-B)(B-i)^{-1},V_2,V_3,\ldots,\tilde{V}_n) \\
=& \mathbf{T}^{H_0,A,B,H_2,\ldots,H_n}_{f^{[n+1]},\{2\}}(V_1,A-B,V_2,V_3,\ldots,\tilde{V}_n) \\
=& \mathbf{T}^{H_0,A,B,H_2,\ldots,H_n}_{f^{[n+1]},\{2,n+1\}}(V_1,A-B,V_2,V_3,\ldots,\tilde{V}_n) \\
=& \mathbf{T}^{H_0,A,B,H_2,\ldots,H_n}_{f^{[n+1]},\{2,n+1\}}(V_1,A-B,V_2,V_3,\ldots,V_n)(H_n-i)^{-1} \\
=:& Y(H_n-i)^{-1},
\end{aligned}
$$

where the second equality is obtained from the first by applying the change of variables (Theorem 47) and using (A.5); the passage from the second to the third equality follows directly from Definition 9 together with the identity

$$
f^{[n+1]}(\lambda_0,\lambda_1,\ldots,\lambda_{n+1})u(\lambda_2) = (fu)^{[n+1]}(\lambda_0,\ldots,\lambda_{n+1}) - (f)^{[n]}(\lambda_0,\lambda_1,\lambda_3,\ldots,\lambda_{n+1}),
$$

while the passage from the third to the fourth equality, as well as from the fourth to the last, proceeds analogously to the argument used for (A.4), namely by invoking Definition 9 and Lemma 10. As $\operatorname{ran}(H_n-i)^{-1} = \operatorname{dom} H_n$ lies dense in $\mathcal{H}$, and since the operators X and Y in front of $(H_n-i)^{-1}$ on the left-hand side and right-hand side are bounded, we obtain the proposition. □

The above proposition serves as the induction basis in the inductive proof of the following result, which is an important component in the proof of our main theorems.

Theorem 50. *Let $n \in \mathbb{N}$ and $j \in \{0,\ldots,n\}$. Let $H_0,\ldots,H_n$ be self-adjoint, and let $V_1,\ldots,V_n$ be operators. Let $\mathcal{J} \subseteq \{1,\ldots,n\}$ be a subset with $n \in \mathcal{J}$ so that V_k is bounded for each $k \in \{1,\ldots,n\} \setminus \mathcal{J}$ and V_k is relatively H_k-bounded for each $k \in \mathcal{J}$. Let W be symmetric and relatively H_j-bounded with H_j-bound < 1. If $j > 0$, suppose that V_j is relatively $H_j + W$-bounded (e.g., $W = tV_j$ for $t \in (-\frac{1}{a},\frac{1}{a})$). For all $f \in \mathscr{W}^{n+1}_{|\mathcal{J}|+1}(\mathbb{R})$ we have*

$$
\begin{aligned}
&\mathbf{T}^{H_0,\ldots,H_{j-1},H_j+W,H_{j+1},\ldots,H_n}_{f^{[n]},\mathcal{J}}(V_1,\ldots,V_n) - \mathbf{T}^{H_0,\ldots,H_n}_{f^{[n]},\mathcal{J}}(V_1,\ldots,V_n) \\
&\qquad = \mathbf{T}^{H_0,\ldots,H_{j-1},H_j+W,H_j,\ldots,H_n}_{f^{[n+1]},p_{j+1}(\mathcal{J})\cup\{j+1\}}(V_1,\ldots,V_j,W,V_{j+1},\ldots,V_n), \quad \text{(A.7)}
\end{aligned}
$$

where $p_{j+1} : \{1, \dots, n\} \to \{1, \dots, n+1\}$ *is defined by* $k \mapsto k$ *for* $k \le j$ *and* $k \mapsto k+1$ *for* $k > j$.

Proof. We prove this by induction to the number of elements in $\mathcal{J}$. The induction basis, $\mathcal{J} = \{n\}$, is Proposition 49.

For the induction step, we choose $k \in \mathcal{J} \setminus \{n\}$. Suppose first that $k \neq j$. In fact, let us assume that $k = 1$ for notational simplicity, because the general proof is precisely the same.

By Lemma 4, from $f \in \mathscr{W}^{n+1}_{|\mathcal{J}|+1}(\mathbb{R})$ it follows that $fu \in \mathscr{W}^{n+1}_{|\mathcal{J}|}(\mathbb{R})$ and $f \in \mathscr{W}^{n}_{|\mathcal{J}|}(\mathbb{R})$. Theorem 48 therefore implies

$$
\begin{aligned}
&\mathbf{T}^{H_0,\dots,H_{j-1},H_j+W,H_{j+1},\dots,H_n}_{f^{[n]},\mathcal{J}}(V_1,\dots,V_n) - \mathbf{T}^{H_0,\dots,H_n}_{f^{[n]},\mathcal{J}}(V_1,\dots,V_n)\\
&= \mathbf{T}^{H_0,\dots,H_{j-1},H_j+W,H_{j+1},\dots,H_n}_{(fu)^{[n]},\mathcal{J}\setminus\{1\}}(V_1(H_1-i)^{-1}, V_2,\dots,V_n)\\
&\quad - \mathbf{T}^{H_0,H_2,\dots,H_{j-1},H_j+W,H_{j+1},\dots,H_n}_{f^{[n-1]},p_1^{-1}(\mathcal{J})}(V_1(H_1-i)^{-1}V_2, V_3,\dots,V_n)\\
&\quad - \mathbf{T}^{H_0,\dots,H_n}_{(fu)^{[n]},\mathcal{J}\setminus\{1\}}(V_1(H_1-i)^{-1}, V_2,\dots,V_n)\\
&\quad + \mathbf{T}^{H_0,H_2,\dots,H_n}_{f^{[n-1]},p_1^{-1}(\mathcal{J})}(V_1(H_1-i)^{-1}V_2, V_3,\dots,V_n)\\
&= \Big(\mathbf{T}^{H_0,\dots,H_{j-1},H_j+W,H_{j+1},\dots,H_n}_{(fu)^{[n]},\mathcal{J}\setminus\{1\}}(V_1(H_1-i)^{-1}, V_2,\dots,V_n)\\
&\qquad - \mathbf{T}^{H_0,\dots,H_n}_{(fu)^{[n]},\mathcal{J}\setminus\{1\}}(V_1(H_1-i)^{-1}, V_2,\dots,V_n)\Big)\\
&\quad - \Big(\mathbf{T}^{H_0,H_2,\dots,H_{j-1},H_j+W,H_{j+1},\dots,H_n}_{f^{[n-1]},p_1^{-1}(\mathcal{J})}(V_1(H_1-i)^{-1}V_2, V_3,\dots,V_n)\\
&\qquad - \mathbf{T}^{H_0,H_2,\dots,H_n}_{f^{[n-1]},p_1^{-1}(\mathcal{J})}(V_1(H_1-i)^{-1}V_2, V_3,\dots,V_n)\Big)
\end{aligned}
\tag{A.8}
$$

We apply the induction hypothesis (two times) to the right-hand side of (A.8), and obtain

$$
\begin{aligned}
&\mathbf{T}^{H_0,\dots,H_{j-1},H_j+W,H_{j+1},\dots,H_n}_{f^{[n]},\mathcal{J}}(V_1,\dots,V_n) - \mathbf{T}^{H_0,\dots,H_n}_{f^{[n]},\mathcal{J}}(V_1,\dots,V_n)\\
&= \mathbf{T}^{H_0,\dots,H_{j-1},H_j+W,H_j,\dots,H_n}_{(fu)^{[n+1]},p_{j+1}(\mathcal{J}\setminus\{1\})\cup\{j+1\}}(V_1(H_1-i)^{-1}, V_2,\dots,V_j,W,V_{j+1},\dots,V_n)\\
&\quad - \mathbf{T}^{H_0,H_2,\dots,H_{j-1},H_j+W,H_j,\dots,H_n}_{f^{[n-1]},p_j(p_1^{-1}(\mathcal{J}))\cup\{j\}}(V_1(H_1-i)^{-1}V_2, V_3,\dots,V_j,W,V_{j+1},\dots,V_n)\\
&= \mathbf{T}^{H_0,\dots,H_{j-1},H_j+W,H_j,\dots,H_n}_{f^{[n+1]},p_{j+1}(\mathcal{J})\cup\{j+1\}}(V_1,\dots,V_j,W,V_{j+1},\dots,V_n),
\end{aligned}
$$

where we have applied Theorem 48 again in the last step, this time using $f \in \mathscr{W}^{n+1}_{|\mathcal{J}|+1}(\mathbb{R})$, as $|p_{j+1}(\mathcal{J}) \cup \{j+1\}| = |\mathcal{J}| + 1$.

We now handle the case $k = j$. We may assume that $\mathcal{J} = \{j, n\}$ without loss of generality; this can be achieved if in the induction process we remove elements $k \neq j$ from $\mathcal{J} \setminus \{n\}$ until we end up with $\mathcal{J} = \{j, n\}$. Again, for purely notational simplicity, we assume that $k = j = 1$.

In the following, the first identity is obtained by applying Theorem 48 (twice, using $f \in \mathscr{W}^n_{|\mathcal{J}|}(\mathbb{R})$). The passage from the first to the second identity, and from the second to the third, consists of straightforward algebraic rearrangements of the initial expression. The transition from the third to the fourth identity follows from Lemma 7 (the second resolvent identity). The fourth-to-fifth identity is derived using Proposition 49 (using $fu \in \mathscr{W}^{n+1}_{|\mathcal{J}|}(\mathbb{R})$) together with Theorem 48 (using $f \in \mathscr{W}^n_{|\mathcal{J}|}(\mathbb{R})$). Finally, the last identity follows from the fifth by another application of Theorem 48(using $f \in \mathscr{W}^{n+1}_{|\mathcal{J}|+1}(\mathbb{R})$).

$$
\begin{aligned}
&\mathbf{T}^{H_0,H_1+W,H_2,\dots,H_n}_{f^{[n]},\{1,n\}}(V_1,\dots,V_n) - \mathbf{T}^{H_0,\dots,H_n}_{f^{[n]},\{1,n\}}(V_1,\dots,V_n)\\
&= \mathbf{T}^{H_0,H_1+W,H_2,\dots,H_n}_{(fu)^{[n]},\{n\}}(V_1(H_1+W-i)^{-1},V_2,\dots,V_n)\\
&\qquad\qquad - \mathbf{T}^{H_0,H_2,\dots,H_n}_{f^{[n-1]},\{n-1\}}(V_1(H_1+W-i)^{-1}V_2,V_3,\dots,V_n)\\
&\quad - \mathbf{T}^{H_0,\dots,H_n}_{(fu)^{[n]},\{n\}}(V_1(H_1-i)^{-1},V_2,\dots,V_n)\\
&\quad + \mathbf{T}^{H_0,H_2,\dots,H_n}_{f^{[n-1]},\{n-1\}}(V_1(H_1-i)^{-1}V_2,V_3,\dots,V_n)\\
&= \mathbf{T}^{H_0,H_1+W,H_2,\dots,H_n}_{(fu)^{[n]},\{n\}}(V_1(H_1+W-i)^{-1},V_2,\dots,V_n)\\
&\quad - \mathbf{T}^{H_0,\dots,H_n}_{(fu)^{[n]},\{n\}}(V_1(H_1-i)^{-1},V_2,\dots,V_n)\\
&\quad - \mathbf{T}^{H_0,H_2,\dots,H_n}_{f^{[n-1]},\{n-1\}}(V_1(H_1+W-i)^{-1}V_2,V_3,\dots,V_n)\\
&\quad + \mathbf{T}^{H_0,H_2,\dots,H_n}_{f^{[n-1]},\{n-1\}}(V_1(H_1-i)^{-1}V_2,V_3,\dots,V_n)\\
&= \mathbf{T}^{H_0,H_1+W,H_2,\dots,H_n}_{(fu)^{[n]},\{n\}}(V_1(H_1+W-i)^{-1},V_2,\dots,V_n)\\
&\quad - \mathbf{T}^{H_0,\dots,H_n}_{(fu)^{[n]},\{n\}}(V_1(H_1+W-i)^{-1},V_2,\dots,V_n)\\
&\quad + \mathbf{T}^{H_0,\dots,H_n}_{(fu)^{[n]},\{n\}}(V_1(H_1+W-i)^{-1}-V_1(H_1-i)^{-1},V_2,\dots,V_n)\\
&\quad - \mathbf{T}^{H_0,H_2,\dots,H_n}_{f^{[n-1]},\{n-1\}}(V_1(H_1+W-i)^{-1}V_2-V_1(H_1-i)^{-1}V_2,V_3,\dots,V_n)\\
&= \mathbf{T}^{H_0,H_1+W,H_2,\dots,H_n}_{(fu)^{[n]},\{n\}}(V_1(H_1+W-i)^{-1},V_2,\dots,V_n)\\
&\quad - \mathbf{T}^{H_0,\dots,H_n}_{(fu)^{[n]},\{n\}}(V_1(H_1+W-i)^{-1},V_2,\dots,V_n)\\
&\quad - \mathbf{T}^{H_0,\dots,H_n}_{(fu)^{[n]},\{n\}}(V_1(H_1+W-i)^{-1}W(H_1-i)^{-1},V_2,\dots,V_n)\\
&\quad + \mathbf{T}^{H_0,H_2,\dots,H_n}_{f^{[n-1]},\{n-1\}}(V_1(H_1+W-i)^{-1}W(H_1-i)^{-1}V_2,V_3,\dots,V_n)\\
&= \mathbf{T}^{H_0,H_1+W,H_1,\dots,H_n}_{(fu)^{[n+1]},\{2,n+1\}}(V_1(H_1+W-i)^{-1},W,V_2,\dots,V_n)\\
&\quad - \mathbf{T}^{H_0,\dots,H_n}_{f^{[n]},\{1,n\}}(V_1(H_1+W-i)^{-1}W,V_2,\dots,V_n)\\
&= \mathbf{T}^{H_0,H_1+W,H_1,\dots,H_n}_{f^{[n+1]},\{1,2,n+1\}}(V_1,W,V_2,\dots,V_n),
\end{aligned}
$$

concluding the proof. □

Data availability

No data was used for the research described in the article.

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