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ON HILBERT–SCHMIDT COMPATIBILITY

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Abstract. Guided by important examples of differential operators, we obtain sufficient conditions for Hilbert-Schmidt compatibility of operators and apply these conditions in spectral perturbation theory.

1. Introduction

The problem for which self-adjoint operators H_0 and H acting on a separable Hilbert space and which scalar functions f, the difference $f(H)-f(H_0)$ of the respective operator functions is in the Schatten-von Neumann ideal S_p has been topical in perturbation theory for over 60 years. The case when the perturbation $V=H-H_0$ belongs to a trace ideal has been well explored; it is known that $V\in S_p$ implies $f(H)-f(H_0)\in S_p$ for any Lipschitz f if $p\in(1,\infty)$ [18] and for any f in the Besov class $\tilde{B}^1_{\infty,1}$ if $p\in\{1,\infty\}$ [12, 13]. One of the questions considered in this paper is for what bounded (non-Hilbert-Schmidt) perturbations V and for what f, we have $(f(H_0+V)-f(H_0))V\in S_1$. Non-Hilbert-Schmidt perturbations and the expressions $\mathrm{tr}\,[(f(H_0+V)-f(H_0))V]$ naturally arise in the study of differential operators, but they are barely explored. We show that certain Hilbert-Schmidt compatibility conditions suffice for $(f(H_0+V)-f(H_0))V$ to be in the trace class and for spectral shift functions to exist.

Given an initial self-adjoint operator $H_0=H_0^*$ in a separable Hilbert space, we say that a family $\mathscr{A}_0$ of (non-Hilbert-Schmidt) perturbations is Hilbert-Schmidt compatible with the operator H_0 in the weak sense if $\phi(H_0+V_1)V_2$ is Hilbert-Schmidt, for all $V_1=V_1^*, V_2=V_2^*\in\mathscr{A}_0$ and all ϕ in some set $\mathfrak{F}$ of smooth functions decaying at infinity (rigorous definitions are given in Section 3). If, in addition, we have continuity of the maps $(V_1,V_2)\mapsto\phi(H_0+V_1)V_2$ in the Hilbert-Schmidt norm, we say that $\mathscr{A}_0$ is Hilbert-Schmidt compatible with H_0. We show that the Hilbert-Schmidt compatibility for a family $\mathfrak{F}$ follows from the compatibility for one simple function (see Theorems 3.4 and 3.5). This result is a partial replacement of the invariance principle for trace class compatible perturbations. We also show that the compatibility in the weak sense often

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implies the (regular) compatibility for a somewhat smaller set of admissible functions $\mathfrak{F}$ (see Theorem 3.5 and theorems of Section 5).

The weak compatibility condition $(1+H_0^2)^{-1/4}V \in S_2$ was considered in [9]. It was shown in [9] that under this condition the operators H_0 and V satisfy Koplienko's trace formula

$$\tau\left[f(H_0+V)-f(H_0)-\frac{d}{dr}f(H_0+rV)\bigg|_{r=0}\right]=\int_{\mathbb{R}} f''(t)\eta(t)\,dt, \tag{1.1}$$

for f any rational function with non-real poles. Here τ is the standard trace on $\mathcal{B}(\mathcal{H})$ and η is a locally integrable function depending only on the operators H_0 and V; it is called Koplienko's spectral shift function (SSF) (for properties of Koplienko's SSF see, e.g., Subsection 4.1.) Koplienko's SSF was introduced as a generalization of Krein's SSF [10]; the former is defined for Schrödinger operators with some long-range potentials (namely, V is a multiplication by a measurable function on $\mathbb{R}^n$ decaying as $\|\vec{x}\|^{-\alpha}$, $\|\vec{x}\| \to \infty$, with $\frac{n}{2} < \alpha \leqslant n$; see discussion in Section 5) while the latter is defined only in the case of short range potentials ($\alpha > n$).

Our main results are discussed in Section 4. We extend the trace formula (1.1) to a broader set of functions f (see Theorems 4.5 and 4.7 and Corollary 4.8) and derive an analogous formula for a more general weak compatibility condition of $(1+H_0^2)^{-1/2}V$ belong to the Hilbert-Schmidt class (see Theorems 4.9 and 4.10). The latter is achieved by replacing the left hand side in (1.1) with $\int_0^1 \tau\big[(f'(H_0+rV)-f'(H_0))V\big]\,dr$, which we show to be well defined in more general situations (see Theorem 3.7) and which coincides with the left hand side in (1.1) when Koplienko's weak compatibility condition is fulfilled. Examples of functions f for which our results hold are given in Lemmas 2.10, 2.11, and 2.12. When the operators H_0 and V are trace class compatible (in the sense of [1]), the generalized Koplienko's SSF considered in this paper can be expressed in terms of the generalized Krein's SSF of [1] (see Lemma 4.11).

Our proofs are based on multiple operator integration techniques derived in Section 2 for Hilbert-Schmidt compatible operators. Our method also applies to τ-Hilbert-Schmidt compatible pairs of operators (see Definitions 3.1 and 3.2), where τ is a normal faithful semi-finite trace defined on a semi-finite von Neumann algebra $\mathcal{M}$ of (bounded) operators acting on a separable Hilbert space $\mathcal{H}$. In this case, V is taken to be an element in $\mathcal{M}$ and H_0 is affiliated with $\mathcal{M}$.

In Section 5, we demonstrate that the initial operators taken to be fractional powers of Laplacians and perturbations taken to be multiplications by bounded L_2-functions satisfy the compatibility condition with $(1+H_0^2)^{-1/2}V$ being in the Hilbert-Schmidt ideal in both the standard and von Neumann algebra settings. Note that assumptions of the type that $(1+H_0^2)^{-1/2}V$ is τ-compact and satisfies some summability condition are of special importance in noncommutative geometry (see e.g. [6]). Examples and detailed treatment of pseudodifferential operators can be found in [5].

Let $L_\alpha(\mathcal{M},\tau)$ denote the noncommutative L_α-space with respect to $(\mathcal{M},\tau)$ and $\mathcal{L}_\alpha(\mathcal{M},\tau)$ the τ-Schatten-von Neumann ideal $L_\alpha(\mathcal{M},\tau)\cap\mathcal{M}$ (see, e.g., [2, 16] for basic definitions and facts), which coincides with the standard Schatten-von Neumann ideal of order α when τ is the standard trace. We denote the norm on $L_\alpha(\mathcal{M},\tau)$ by $\|V\|_\alpha := \tau(|V|^\alpha)^{1/\alpha}$ and the norm on $\mathcal{L}_\alpha(\mathcal{M},\tau)$ by $\|\cdot\|_{\alpha\cap\infty} := \|\cdot\|_\alpha + \|\cdot\|_\infty$, for

$1 \leqslant \alpha \leqslant \infty$. Here $\|\cdot\|_\infty$ coincides with the operator norm. Since the algebra $\mathscr{M}$ and the trace τ are fixed throughout this paper, we omit $(\mathscr{M},\tau)$ from the notation $L_\alpha(\mathscr{M},\tau)$ and $\mathscr{L}_\alpha(\mathscr{M},\tau)$ and write simply L_α and $\mathscr{L}_\alpha$, respectively.

2. Multiple operator integrals

In this section, we study properties of multiple operator integrals for Hilbert-Schmidt compatible operators.

2.1. Basic properties.

First, we recall the definition of a multiple operator integral due to [2, 15]. Let $\mathfrak{A}^n$ be the class of functions $\phi:\mathbb{R}^{n+1}\mapsto\mathbb{C}$ admitting the representation

$$\phi(\lambda_0,\dots,\lambda_n)=\int_\Omega\prod_{j=0}^n a_j(\lambda_j,s)\,d\mu(s), \tag{2.1}$$

for some finite measure space (Ω,μ) and bounded Borel functions $a_j:\mathbb{R}\times\Omega\mapsto\mathbb{C}$ satisfying $\int_\Omega\prod_{j=0}^n\left\|a_j(\cdot,s)\right\|_\infty d|\mu|(s)<\infty$. The class $\mathfrak{A}^n$ has the norm

$$\|\phi\|_{\mathfrak{A}^n}:=\inf\int_\Omega\prod_{j=0}^n\left\|a_j(\cdot,s)\right\|_\infty d|\mu|(s),$$

where the infimum is taken over all possible representations (2.1). We will work with the subclass $\mathfrak{C}^n\subset\mathfrak{A}^n$ of functions $\phi:\mathbb{R}^{n+1}\mapsto\mathbb{C}$ admitting the representation (2.1) with bounded continuous functions

$$a_j(\cdot,s):\mathbb{R}\mapsto\mathbb{C},$$

for which there is a growing sequence of measurable subsets $\{\Omega_k\}_{k\geqslant1}$, with $\Omega_k\subseteq\Omega$ and $\cup_{k\geqslant1}\Omega_k=\Omega$, such that the families

$$\left\{a_j(\cdot,s)\right\}_{s\in\Omega_k},\quad 0\leqslant j\leqslant n,$$

are uniformly bounded and uniformly equicontinuous and given $\varepsilon>0$, $\exists k_\varepsilon\in\mathbb{N}$, for which

$$\int_{\Omega\setminus\Omega_{k_\varepsilon}}\prod_{j=0}^n\|a_j(\cdot,s)\|_\infty d|\mu|(s)<\varepsilon.$$

DEFINITION 2.1. Let $H_0,\dots,H_n$ be (possibly unbounded) self-adjoint operators in $\mathscr{H}$ and $V_1,\dots,V_n$ bounded self-adjoint operators on $\mathscr{H}$. For $\phi\in\mathfrak{A}^n$, the multiple operator integral $T_\phi^{H_0,\dots,H_n}(V_1,\dots,V_n)$ is an operator defined for every $y\in\mathscr{H}$ as the Bochner integral

$$T_\phi^{H_0,\dots,H_n}(V_1,\dots,V_n)y:=\int_\Omega a_0(H_0,s)V_1a_1(H_1,s)\dots V_na_n(H_n,s)y\,d\mu(s).$$

It was shown in [15, Lemma 3.1] (cf. also [2, Lemma 4.3]) that this definition is independent of the choice of the representation (2.1).

We are particularly interested in the cases $n=1$ and $n=2$. The theory of double operator integrals (the case $n=1$) was initiated by Yu. L. Daletskii and S.G. Krein and greatly expanded and elaborated by M. Birman and M. Solomyak (see, e.g., [4]).

We have the following estimate for the multiple operator integral.

PROPOSITION 2.2. (See [2, Lemma 3.5 and Remark 4.2].) *Let $1 \leqslant \alpha_j \leqslant \infty$, with $1 \leqslant j \leqslant n$, be such that $0 \leqslant \frac{1}{\alpha} := \frac{1}{\alpha_1} + \ldots + \frac{1}{\alpha_j} \leqslant 1$. Let $H_0 = H_0^*$ be affiliated with $\mathscr{M}$ and $V_j = V_j^* \in \mathscr{L}_{\alpha_j}$, for $j \in \{1, \ldots, n\}$. For every $\phi \in \mathfrak{A}^n$,*

$$\left\| T_\phi^{H_0,\ldots,H_n}(V_1,\ldots,V_n) \right\|_\alpha \leqslant \|\phi\|_{\mathfrak{A}^n} \|V_1\|_{\alpha_1} \cdots \|V_n\|_{\alpha_n}. \tag{2.2}$$

REMARK 2.3. The transformation $T_\phi^{H_0,\ldots,H_n}$ admits a unique bounded extension from $\mathscr{L}_{\alpha_1} \times \ldots \times \mathscr{L}_{\alpha_n}$ to $L_{\alpha_1} \times \ldots \times L_{\alpha_n}$ with preservation of the bound (2.2).

The main application of multiple operator integration lies in perturbation theory. In this case, divided differences come into play.

DEFINITION 2.4. The divided difference of order n is an operation on functions $f \in C^n(\mathbb{R})$ of one (real) variable, which we will usually call λ, defined recursively as follows:

$$f^{[0]}(\lambda_0) := f(\lambda_0),$$

$$f^{[n]}(\lambda_0,\ldots,\lambda_{n-2},\lambda_{n-1},\lambda_n) := \begin{cases} \frac{f^{[n-1]}(\lambda_0,\ldots,\lambda_{n-2},\lambda_{n-1}) - f^{[n-1]}(\lambda_0,\ldots,\lambda_{n-2},\lambda_n)}{\lambda_{n-1}-\lambda_n} & \text{if } \lambda_{n-1} \neq \lambda_n \\ \frac{\partial}{\partial t}\Big|_{t=\lambda_n} f^{[n-1]}(\lambda_0,\ldots,\lambda_{n-2},t) & \text{if } \lambda_{n-1} = \lambda_n. \end{cases}$$

Observe that, for $\{\lambda_0,\ldots,\lambda_n\} \subset [a,b]$,

$$\left| f^{[n]}(\lambda_0,\ldots,\lambda_n) \right| \leqslant \frac{1}{n!} \max_{\lambda \in [a,b]} |f^{(n)}(\lambda)|. \tag{2.3}$$

We also have an analog of the Leibnitz differentiation formula

$$(gh)^{[n]}(\lambda_0,\ldots,\lambda_n) = \sum_{k=0}^{n} g^{[k]}(\lambda_0,\ldots,\lambda_k) h^{[n-k]}(\lambda_k,\ldots,\lambda_n), \quad \text{for } g,h \in C^n(\mathbb{R}). \tag{2.4}$$

Let $\tilde{B}^n_{\infty,1}$ denote the modified homogeneous Besov class on $\mathbb{R}$ (see definition in [15]) and Λ_γ the Hölder class of order $\gamma \geqslant 0$. Recall that Λ_γ is the set of functions f for which

$$\|f\|_{\Lambda_\gamma} := \sup_{t_1,t_2} \frac{|f(t_1)-f(t_2)|}{|t_1-t_2|^\gamma} < \infty.$$

In general it may be difficult to see if a function belongs to the class $\tilde{B}^n_{\infty,1}$. The following proposition however delivers several "easier to test" subclasses of $\tilde{B}^n_{\infty,1}$.

PROPOSITION 2.5. *A function $f \in C^n(\mathbb{R})$ belongs to $\tilde{B}^n_{\infty,1}$ if either of the following conditions is satisfied.*

(i) $\widehat{f^{(n)}} \in L_1(\mathbb{R})$;

(ii) $f^{(n-1)} \in \Lambda_{1-\varepsilon}$ *and* $f^{(n)} \in \Lambda_\varepsilon$ *for some* $0 < \varepsilon \leqslant 1$;

(iii) $f^{(n)} \in L_2(\mathbb{R})$ *and* $f^{(n+1)} \in L_2(\mathbb{R})$.

Proof. The first claim directly follows from the construction of the classes $\tilde{B}^n_{\infty,1}$; the second claim, in the special case $n = 1$, is proved in [20, Theorem 4 and Remark 5], the general case can be proved analogously; the last claim easily follows from the first one and the observation that every L_2-function with L_2-derivative has integrable Fourier transform (see [20, Lemma 7] for details). □

The next result follows from a careful analysis of [15, Theorem 5.5].

PROPOSITION 2.6. *If $f \in \tilde{B}^n_{\infty,1}$, then $f^{[n]} \in \mathfrak{C}^n$.*

To expand the sphere of applicability of our results, we consider one more construction of a multiple operator integral which does not require a tensor product decomposition of a function ϕ as in (2.1). In this construction [19], multiple operator integrals are represented as limits of Riemann sums with admissible partitions.

Let E_H denote the spectral measure of H. We set $E_{H,l,m} := E_H\left(\left[\frac{l}{m}, \frac{l+1}{m}\right)\right)$, for every $m \in \mathbb{N}$ and $l \in \mathbb{Z}$. Let $\phi : \mathbb{R}^n \mapsto \mathbb{C}$ be a bounded continuous function. In case of convergence, denote

$$\hat{T}_\phi^{H_0,\dots,H_n}(V_1,\dots,V_n)$$

$$:= \text{SOT-}\lim_{m\to\infty} \|\cdot\|_\alpha\text{-}\lim_{N\to\infty} \sum_{|l_0|,\dots,|l_n|\leqslant N} \phi\left(\frac{l_0}{m},\dots,\frac{l_n}{m}\right) E_{H_0,l_0,m}V_1E_{H_1,l_1,m}V_2\dots V_nE_{H_n,l_n,m},$$

where the first limit gives bounded polylinear operators and the second one is evaluated in the strong operator topology on the tuples $(V_1,\dots,V_n) \in L_{\alpha_1} \times \dots \times L_{\alpha_n}$, where $\frac{1}{\alpha_1} + \dots + \frac{1}{\alpha_n} = \frac{1}{\alpha}$. Note that the values of the function ϕ outside the set $(a,b)^n$, where the interval (a,b) contains the spectra of $H_0,\dots,H_n$, do not affect the values of $\hat{T}_\phi$.

PROPOSITION 2.7. (See [19, Lemma 3.5].) *Let $1 \leqslant \alpha_j \leqslant \infty$, with $1 \leqslant j \leqslant n$, be such that $0 \leqslant \frac{1}{\alpha} := \frac{1}{\alpha_1} + \dots + \frac{1}{\alpha_j} \leqslant 1$. Let $H_0 = H_0^*$ be affiliated with $\mathscr{M}$ and $V_j = V_j^* \in L_{\alpha_j}$, for $j \in \{1,\dots,n\}$. For every $\phi \in \mathfrak{C}^n$, $\hat{T}_\phi^{H_0,\dots,H_0}(V_1,\dots,V_n)$ is a bounded polylinear operator mapping $L_{\alpha_1} \times \dots \times L_{\alpha_n} \mapsto L_\alpha$. Moreover, $\hat{T}_\phi^{H_0,\dots,H_0}(V_1,\dots,V_n)$ coincides with $T_\phi^{H_0,\dots,H_0}(V_1,\dots,V_n)$ given by Definition 2.1.*

Observe that $\|E_{H_0,l_0,m}VE_{H_1,l_1,m}\|_2^2 = \tau(E_{H_0,l_0,m}VE_{H_1,l_1,m}V)$ whenever $V \in L_2$. Since $\{E_{H_i,l_i,m}\}_{l_i}$ is a family of mutually orthogonal projections, $i = 0,1$, we have

$$\left\| \sum_{|l_0|,|l_1|\leqslant N} \phi\left(\frac{l_0}{m},\frac{l_1}{m}\right) E_{H_0,l_0,m}VE_{H_1,l_1,m} \right\|_2^2 \leqslant \|\phi\|_\infty^2 \,\tau\left(\sum_{|l_0|\leqslant N} E_{H_0,l_0,m}V \sum_{|l_1|\leqslant N} E_{H_1,l_1,m}V \right).$$

Consequently, it can be readily seen that $\hat{T}_{\phi}^{H_0,H_1}(V)$ is well defined for every bounded continuous ϕ and

$$\left\|\hat{T}_{\phi}^{H_0,H_1}(V)\right\|_2 \leqslant \|\phi\|_\infty \|V\|_2. \tag{2.5}$$

The estimate (2.5) is classical; it goes back to the original work by Birman and Solomyak on double operator integrals in the 1960s.

We have the following continuity properties of the multiple operator integrals. Let $C_b^1(\mathbb{R})$ be the space of all bounded continuously differentiable functions with bounded derivative.

LEMMA 2.8. *(i) Let $\{H_{i,n}\}_n$ be a sequence of self-adjoint operators affiliated with $\mathscr{M}$ and converging to H_i, $i=0,1,2$, in the strong resolvent sense and let $V_1,V_2\in\mathscr{L}_2$. Then, for every $\phi\in\mathfrak{C}^2$,*

$$\lim_{n\to\infty}\left\|T_{\phi}^{H_{0,n},H_{1,n},H_{2,n}}(V_1,V_2)-T_{\phi}^{H_0,H_1,H_2}(V_1,V_2)\right\|_1=0$$

and, for every $\phi\in\mathfrak{C}^1$,

$$\lim_{n\to\infty}\left\|T_{\phi}^{H_{0,n},H_{1,n}}(V_1)V_2-T_{\phi}^{H_0,H_1}(V_1)V_2\right\|_1=0.$$

(ii) Let $H_i=H_i^*$, $i=0,1,2$, be affiliated with $\mathscr{M}$ and let $\{V_{j,n}\}_n$ be a sequence of self-adjoint operators in $\mathscr{L}_2$ converging to a bounded self-adjoint operator V_j in the L_2-norm, $j=1,2$. Then, for every $\phi\in\mathfrak{A}^2$,

$$\lim_{n\to\infty}\left\|T_{\phi}^{H_0,H_1,H_2}(V_{1,n},V_{2,n})-T_{\phi}^{H_0,H_1,H_2}(V_1,V_2)\right\|_1=0.$$

(iii) Let $\{f_n\}_n\cup\{f\}\subset C_b^1(\mathbb{R})$ be such that $\{f_n'\}_n$ converges to f' in the supremum norm. Then, for any $V_1=V_1^*,V_2=V_2^*\in\mathscr{L}_2$ and any $H_0=H_0^*,H_1=H_1^*$ affiliated with $\mathscr{M}$,

$$\lim_{n\to\infty}\tau\left(\hat{T}_{f_n^{[1]}}^{H_0,H_1}(V_1)V_2\right)=\tau\left(\hat{T}_{f^{[1]}}^{H_0,H_1}(V_1)V_2\right).$$

Proof. (i) The functions $a_j(\cdot,s)$ from the decomposition (2.1) are continuous and bounded (uniformly in s), so the sequence $\{a_i(H_{n,i},s)\}_n$ converges to $a_i(H_i,s)$ in the strong operator topology for every $s\in\Omega$, $i=0,1,2$ [21, Theorem VIII.20 (b)]. Since V_1 and V_2 are bounded, we have that, for any $s\in\Omega$,

$$\|\cdot\|_1\text{-}\lim_{n\to\infty}a_0(H_{n,0},s)V_1a_1(H_{n,1},s)V_2a_2(H_{n,2},s)=a_0(H_0,s)V_1a_1(H_1,s)V_2a_2(H_2,s).$$

We also have

$$\sup_n\|a_0(H_{n,0},\cdot)V_1a_1(H_{n,1},\cdot)V_2a_2(H_{n,2},\cdot)\|_1\in L_1(\Omega,\mu).$$

Therefore, by the Lebesgue dominated convergence theorem for Bochner integrals, we have the convergence of multiple operator integrals.

(ii) The proof follows from the estimate (2.2).

(iii) Observe that by the definition, we have

$$\hat{T}^{H_0,H_1}_{f_n^{[1]}}(V_1) - \hat{T}^{H_0,H_1}_{f^{[1]}}(V_1) = \hat{T}^{H_0,H_1}_{f_n^{[1]}-f^{[1]}}(V_1).$$

Next, via (2.5),

$$\left\| \hat{T}^{H_0,H_1}_{f_n^{[1]}}(V_1) - \hat{T}^{H_0,H_1}_{f^{[1]}}(V_1) \right\|_2 \leqslant \|V_1\|_2 \left\| f_n^{[1]} - f^{[1]} \right\|_\infty .$$

Finally, via (2.3),

$$\left\| f_n^{[1]} - f^{[1]} \right\|_\infty \leqslant \|f_n' - f'\|_\infty \to 0.$$

The proof of the claim now easily follows from the Hölder inequality. □

We have the following perturbation lemma.

LEMMA 2.9. *Let* $H_0,\dots,H_n$ *be self-adjoint operators affiliated with* $\mathscr{M}$ *and* $V_1,\dots,V_n$ *be self-adjoint operators in* $\mathscr{M}$. *Let* $\psi \in L_\infty(\mathbb{R}^{n+1})$, *with* $n \in \{1,2\}$, *and let* $\phi \in C_b(\mathbb{R})$; *denote* $(\psi\phi)(\lambda_0,\dots,\lambda_n) := \psi(\lambda_0,\dots,\lambda_n)\phi(\lambda_1)$. *The following assertions hold.*

(i) If $\hat{T}_\psi$ *exists, then* $\hat{T}_{\psi\phi}$ *exists also and*

$$\hat{T}^{H_0,H_1}_{\psi}(V_1)\phi(H_1) = \hat{T}^{H_0,H_1}_{\psi\phi}(V_1).$$

(ii) If $\psi \in \mathfrak{A}^2$, *then* $\psi\phi \in \mathfrak{A}^2$ *and*

$$T^{H_0,H_1,H_2}_{\psi}(V_1\phi(H_1),V_2) = T^{H_0,H_1,H_2}_{\psi\phi}(V_1,V_2).$$

Proof. The proof is straightforward; we demonstrate only the proof of part (i).

$$\hat{T}^{H_0,H_1}_{\psi}(V_1)\phi(H_1) = \text{SOT-}\lim_{m\to\infty} \|\cdot\|_2\text{-}\lim_{N\to\infty} \sum_{|l_0|,|l_1|\leqslant N} \psi\left(\frac{l_0}{m},\frac{l_1}{m}\right) E_{H_0,l_0,m} V_1 \phi(H_1) E_{H_1,l_1,m}. \tag{2.6}$$

By the spectral theorem,

$$\phi(H_1) = \|\cdot\|_\infty\text{-}\lim_{m\to\infty} \sum_{l\in\mathbb{Z}} \phi\left(\frac{l}{m}\right) E_{H_1,l,m}.$$

Therefore, (2.6) equals

$$\text{SOT-}\lim_{m\to\infty} \|\cdot\|_2\text{-}\lim_{N\to\infty} \sum_{|l_0|,|l_1|\leqslant N} \psi\left(\frac{l_0}{m},\frac{l_1}{m}\right) \phi\left(\frac{l_1}{m}\right) E_{H_0,l_0,m} V_1 E_{H_1,l_1,m} = \hat{T}^{H_0,H_1}_{\psi\phi}(V_1). \quad \square$$

2.2. Weighted divided differences

Now we consider the case of non-Hilbert-Schmidt perturbations V such that $Vg(H_0) \in \mathcal{L}_2$ for some nice function g. This implies consideration of weighted divided differences.

Given $\psi \in C(\mathbb{R})$, let $\mathfrak{C}_\psi^n$ denote the set of all bounded functions $f \in C^n(\mathbb{R})$ such that $f^{[n]}\psi \in \mathfrak{C}^n$, where $n \in \mathbb{N} \cup \{0\}$ and

$$(f^{[n]}\psi)(\lambda_0,\lambda_1,\dots,\lambda_n) := f^{[n]}(\lambda_0,\lambda_1,\dots,\lambda_n)\psi(\lambda_1).$$

Observe that the divided difference $f^{[n]}$ is invariant under any permutation of its variables, so the choice of λ_1 for the factor ψ is not essential. If $\psi^{-1} \in C_b(\mathbb{R})$, then for any $f \in \mathfrak{C}_\psi^n$, we also have $f^{[n]} \in \mathfrak{C}^n$ (the case $n=2$ follows from the assertion of Lemma 2.9 (ii)). Let L_ψ denote the set of functions $f \in C^1(\mathbb{R})$ such that $f^{[1]} \in \mathfrak{C}^1$ and $f^{[1]}\psi \in L_\infty(\mathbb{R}^2)$ (in fact, $f^{[1]}\psi$ is continuous and bounded).

In the next three lemmas, we provide examples of functions in L_ψ and $\mathfrak{C}_\psi^1$.

Let $\mathfrak{R}_b$ denote the set of bounded rational functions with non-real poles and bounded at infinity, $C_c(\mathbb{R})$ the subset of $C(\mathbb{R})$ of compactly supported functions, $C_0(\mathbb{R})$ the subset of $C(\mathbb{R})$ of functions decaying at infinity, and $C_b(\mathbb{R})$ the set of bounded continuous functions. Given a function f without zeros, the symbol f^{-1} denotes the function $t \mapsto \frac{1}{f(t)}$; given an invertible function f, the symbol f_{inv} denotes the inverse of f.

LEMMA 2.10. *For $g(t) = (1+t^s)^\alpha$, where $\alpha \in [-\frac{1}{s},0)$, $s \in 2\mathbb{N}$,*

$$C_c^2(\mathbb{R}) \cup \mathfrak{R}_b \cup \{g\} \subset L_{g^{-1}}.$$

Proof. For any $f,\psi \in C^1(\mathbb{R})$, by (2.4), we have

$$f^{[1]}(\lambda_0,\lambda_1)\psi(\lambda_1) = (f\psi)^{[1]}(\lambda_0,\lambda_1) - f(\lambda_0)\psi^{[1]}(\lambda_0,\lambda_1).$$

Whenever $f,\psi',(f\psi)' \in L_\infty(\mathbb{R})$, applying the estimate (2.3) guarantees $f^{[1]}\psi \in L_\infty(\mathbb{R}^2)$. Let $f \in C_c^2(\mathbb{R}) \cup \mathfrak{R}_b \cup \{g\}$. Taking $\psi = g^{-1}$ completes the proof of the lemma. □

LEMMA 2.11. *For $g(t) = (1+t^s)^\alpha$, where $\alpha \in [-\frac{1}{s},0)$, $s \in 2\mathbb{N}$,*

$$\mathfrak{R}_b \subset \mathfrak{C}_{g^{-1}}^1 \cap \mathfrak{C}_{g^{-1}}^2.$$

Proof. The result follows from the representation for the divided difference of the rational function $f_{k,z}(t) = (z-t)^{-k}$, where $k \in \mathbb{N}$ and $\mathrm{Im} z \neq 0$:

$$f_{k,z}^{[n]}(\lambda_0,\lambda_1,\dots,\lambda_n) = \sum_{\substack{1 \leqslant k_0,k_1,\dots,k_n \leqslant k \\ k_0+k_1+\dots+k_n = k+n}} (z-\lambda_0)^{-k_0}(z-\lambda_1)^{-k_1}\dots(z-\lambda_n)^{-k_n}. \quad (2.7)$$

This representation can be proved by induction on k. Observe that

$$f_{1,z}^{[n]}(\lambda_0,\lambda_1,\dots,\lambda_n)=(z-\lambda_0)^{-1}(z-\lambda_1)^{-1}\dots(z-\lambda_n)^{-1}.$$

Since $f_{k+1,z}=f_{1,z}f_{k,z}$, by (2.4), we obtain

$$f_{k+1,z}^{[n]}(\lambda_0,\dots,\lambda_n)=\sum_{k=0}^{n} f_{1,z}^{[k]}(\lambda_0,\dots,\lambda_k)f_{k,z}^{[n-k]}(\lambda_k,\dots,\lambda_n).$$

If we assume that (2.7) holds, then we can derive that (2.7) holds for k replaced with $k+1$. $\square$

LEMMA 2.12. *Let $f\in C^2(\mathbb{R})$ be such that*

$$\sup_{0\leqslant t,\,0\leqslant k\leqslant 3}|t^{k+\varepsilon}f^{(k)}(t)|<\infty, \tag{2.8}$$

for some $\varepsilon>\frac{1}{2}$. Let $g(t)=(1+t^s)^\alpha$, where $\alpha\in[-\frac{1}{s},0)$, $s\in 2\mathbb{N}$, and let $\psi_\delta\in C^2(\mathbb{R})$ be a function coinciding with $\chi_{[\delta,\infty)}$ on $(-\infty,\delta/2]\cup[\delta,\infty)$, for some $\delta>0$. Then,

$$(\lambda_0,\dots,\lambda_n)\mapsto \phi_{n,\delta}(\lambda_0,\dots,\lambda_n):=f^{[n]}(\lambda_0,\dots,\lambda_n)\prod_{j=0}^{n}\psi_\delta(\lambda_j)\in\mathfrak{C}^n_{g^{-1}}, \tag{2.9}$$

for $n=1,2$.

Proof. In the proof below, we can assume that f is supported in $[\delta/2,\infty)$ since the function in (2.9) coincides with the function

$$(\lambda_0,\dots,\lambda_n)\mapsto (f\psi_{\delta/2})^{[n]}(\lambda_0,\dots,\lambda_n)\prod_{j=0}^{n}\psi_\delta(\lambda_j).$$

Let $\lambda_0,\dots,\lambda_n\geqslant\frac{\delta}{2}$.

Firstly, we consider the case $n=1$. By the Leibnitz formula (2.4),

$$f^{[1]}(\lambda_0,\lambda_1)g^{-1}(\lambda_1)=(fg^{-1})^{[1]}(\lambda_0,\lambda_1)-f(\lambda_0)(g^{-1})^{[1]}(\lambda_0,\lambda_1).$$

The property (2.8) ensures $(fg^{-1})',(fg^{-1})''\in L_2(\mathbb{R})$. Hence, by Propositions 2.5 and 2.6,

$$(fg^{-1})^{[1]}(\lambda_0,\lambda_1)\psi_\delta(\lambda_0)\psi_\delta(\lambda_1)\in\mathfrak{C}^1.$$

By linearity of the divided difference,

$$(g^{-1})^{[1]}(\lambda_0,\lambda_1)=\big(g^{-1}(\lambda)-\lambda^{-\alpha s}\big)^{[1]}(\lambda_0,\lambda_1)+\big(\lambda^{-\alpha s}\big)^{[1]}(\lambda_0,\lambda_1).$$

It is routine to see that the first and second derivatives of $g^{-1}(\lambda)-\lambda^{-\alpha s}$ are in $L_2([\frac{\delta}{2},\infty))$. Thus,

$$\big(g^{-1}(\lambda)-\lambda^{-\alpha s}\big)^{[1]}(\lambda_0,\lambda_1)\psi_\delta(\lambda_0)\psi_\delta(\lambda_1)\in\mathfrak{C}^1.$$

Now we consider the function $h(\lambda) = \lambda^{-\alpha s}$, $\lambda \geqslant \frac{\delta}{2}$. If $-\alpha s = 1$, then $h^{[1]} \equiv 1 \in \mathfrak{C}^1$. If $0 < -\alpha s < 1$, then h', h'' are bounded and $h \in \Lambda_{-\alpha s}$. Hence, by [20, Theorem 4],

$$\left(\lambda^{-\alpha s}\right)^{[1]}(\lambda_0, \lambda_1)\psi_\delta(\lambda_0)\psi_\delta(\lambda_1) \in \mathfrak{C}^1.$$

Therefore, we have established

$$f^{[1]}(\lambda_0, \lambda_1)g^{-1}(\lambda_1)\psi_\delta(\lambda_0)\psi_\delta(\lambda_1) \in \mathfrak{C}^1.$$

The claim (2.9) in case $n = 2$ can be derived from (2.4) by a reasoning completely analogous to the one above. □

2.3. Some perturbation results

Sufficient conditions for the Hilbert-Schmidt compatibility will be derived from the following perturbation results.

LEMMA 2.13. *Let $U = U^*$, $V = V^*$ be elements in $\mathcal{M}$ and $H_0 = H_0^*$ be affiliated with $\mathcal{M}$. If $g \in C_b(\mathbb{R})$ has no zeros and $Ug(H_0) \in \mathcal{L}_2$, then, for $f \in L_{g^{-1}}$,*

$$T^{H_0+V,H_0}_{f^{[1]}}(U) = \hat{T}^{H_0+V,H_0}_{f^{[1]}g^{-1}}(Ug(H_0)) \in \mathcal{L}_2.$$

Proof. Since $f^{[1]}g^{-1} \in C_b(\mathbb{R}^2)$, the proof is an immediate application of Lemma 2.9 and Proposition 2.7. □

LEMMA 2.14. *Let H_0 and H_1 be self-adjoint operators affiliated with $\mathcal{M}$ such that $H_1 - H_0$ extends to a bounded operator in $\mathcal{M}$, also denoted by $H_1 - H_0$. If $f \in C_b(\mathbb{R})$ and $f^{[1]} \in \mathfrak{C}^1$, then*

$$f(H_1) - f(H_0) = T^{H_1,H_0}_{f^{[1]}}(H_1 - H_0). \tag{2.10}$$

Proof. First we prove the lemma under the additional assumption that H_0 and H_1 are bounded. This trivially follows from algebraic properties of operator integrals. Indeed, with employment of Lemma 2.9, we derive

$$\begin{aligned} T_{f^{[1]}}(H_1 - H_0) &= T_{f^{[1]}}(H_1) - T_{f^{[1]}}(H_0) \\ &= T_{F_1}(1) - T_{F_2}(1) = T_{F_1-F_2}(1) = T_{F_3}(1) \\ &= f(H_1) - f(H_0), \quad \text{where } T_F = T_F^{H_1,H_0}, \\ F_1(x,y) = xf^{[1]}(x,y),\ \ & F_2(x,y) = yf^{[1]}(x,y),\ \ F_3(x,y) = f(x) - f(y). \end{aligned}$$

The result for arbitrary operators follows now via approximation. Indeed, let $E_{j,n}$ denote the spectral projection $E_{H_j}((-n,n))$ and let $H_{j,n} := H_jE_{j,n}$. It follows from the bounded version of the lemma that

$$f(H_{1,n}) - f(H_{0,n}) = T^{H_{1,n},H_{0,n}}_{f^{[1]}}(H_{1,n} - H_{0,n}) = E_{1,n}T^{H_1,H_0}_{f^{[1]}}(H_1 - H_0)E_{0,n}.$$

Letting $n \to \infty$, we observe that the left hand side converges in the weak operator topology to $f(H_1) - f(H_0)$ (by [21, Theorems VIII.25.(a) and VIII.20]) and the right hand side converges in the weak operator topology to $T_{f^{[1]}}^{H_1,H_0}(H_1 - H_0)$. Thus, (2.10) holds. □

LEMMA 2.15. *Let g be a function in $C_b(\mathbb{R})$ without zeros. If $H_0 = H_0^*$ is affiliated with $\mathscr{M}$ and $V = V^* \in \mathscr{M}$ is such that $g(H_0)V \in \mathscr{L}_2$, then, for every $f \in L_{g^{-1}}$,*

$$f(H_0+V) - f(H_0) = \hat{T}_{f^{[1]}g^{-1}}^{H_0+V,H_0}(Vg(H_0)).$$

Proof. The result follows from Lemmas 2.14 and 2.13. □

LEMMA 2.16. *Let g be a function in $C_b(\mathbb{R})$ without zeros. If $H_0 = H_0^*$ is affiliated with $\mathscr{M}$, $V = V^* \in \mathscr{M}$, and $g(H_0)V \in \mathscr{L}_2$, then for every $f \in L_{g^{-2}}$,*

$$\big(f(H_0+V) - f(H_0)\big)V = \hat{T}_{f^{[1]}g^{-2}}^{H_0+V,H_0}(Vg(H_0))(g(H_0)V).$$

Proof. Observe that $L_{g^{-2}} \subset L_{g^{-1}}$. It follows from Lemma 2.15 that

$$\begin{aligned}\big(f(H_0+V) - f(H_0)\big)V &= (f(H_0+V) - f(H_0))g^{-1}(H_0)\big(g(H_0)V\big)\\ &= \hat{T}_{f^{[1]}g^{-1}}^{H_0+V,H_0}(Vg(H_0))g^{-1}(H_0)\big(g(H_0)V\big).\end{aligned}$$

Since by Lemma 2.9

$$\hat{T}_{f^{[1]}g^{-1}}^{H_0+V,H_0}(Vg(H_0)) = \hat{T}_{f^{[1]}g^{-2}}^{H_0+V,H_0}\big(Vg(H_0)\big)g(H_0),$$

the result follows. □

Operator derivatives can be expressed as multiple operator integrals.

PROPOSITION 2.17. ([15, Theorem 5.6]) *Let $H_0 = H_0^*$ be defined in $\mathscr{H}$ and $V = V^* \in \mathscr{B}(\mathscr{H})$. Then, for $f \in \tilde{B}_{\infty,1}^n \cap \tilde{B}_{\infty,1}^1$, the function $t \mapsto f(H_0+tV)$ has n-th derivative (in the operator norm)*

$$\frac{d^n}{dt^n} f(H_0+tV)\bigg|_{t=0} = n!\, T_{f^{[n]}}^{H_0,\ldots,H_0}(V,\ldots,V).$$

We will also need the following formula for the first derivative.

LEMMA 2.18. *Let $H_0 = H_0^*$ be affiliated with $\mathscr{M}$ and $V = V^* \in \mathscr{M}$. Let $g \in C_b(\mathbb{R})$ be a function without zeros. If $g(H_0)V \in L_2$, then for $f \in L_{g^{-1}} \cap \mathfrak{C}_{g^{-1}}^2$,*

$$\frac{d}{dt}\left[f(H_0+tV)\right]\bigg|_{t=0} = \hat{T}_{f^{[1]}g^{-1}}^{H_0,H_0}(Vg(H_0)),$$

where the derivative exists in the L_1-norm, that is,

$$\lim_{t\to 0}\left\|\frac{f(H_0+tV) - f(H_0)}{t} - \hat{T}_{f^{[1]}g^{-1}}^{H_0,H_0}(Vg(H_0))\right\|_1 = 0. \tag{2.11}$$

The proof of Lemma 2.18 is based on the algebraic property of operator integrals given below.

LEMMA 2.19. *Let* $H_j = H_j^*,\ j = 0,1$ *be affiliated with* $\mathcal{M}$ *such that*[1] $H_1 - H_0 \in L_2(\mathcal{M},\tau)$ *and let* $V = V^* \in \mathcal{M}$. *Let* $g \in C_b(\mathbb{R})$ *be a function without zeros. If* $g(H_0)V \in L_2$, *then for* $f \in L_{g^{-1}} \cap \mathfrak{C}^2_{g^{-1}}$,

$$\hat{T}^{H_1,H_0}_{f^{[1]}g^{-1}}(Vg(H_0)) - \hat{T}^{H_0,H_0}_{f^{[1]}g^{-1}}(Vg(H_0)) = T^{H_1,H_0,H_0}_{f^{[2]}g^{-1}}(H_1 - H_0, Vg(H_0)),$$

where $(f^{[2]}g^{-1})(\lambda_0,\lambda_1,\lambda_2) := f^{[2]}(\lambda_0,\lambda_1,\lambda_2)g^{-1}(\lambda_2)$.

Proof. We demonstrate the proof only in the case $g \equiv 1$. The proof repeats the lines of that of Lemma 2.14, from which we adopt the notations. In the case of general g, one also needs to apply Lemma 2.13.

We first assume that $H_0, H_1 \in \mathcal{M}$. In this case, the identity is a simple algebraic property of operator integrals. Indeed, with application of Lemma 2.9 and Proposition 2.7,

$$\begin{aligned} T_{f^{[2]}}(H_1 - H_0, V) &= \hat{T}_{f^{[2]}}(H_1 - H_0, V) = \hat{T}_{f^{[2]}}(H_1, V) - \hat{T}_{f^{[2]}}(H_0, V) \\ &= \hat{T}_{F_1}(1,V) - \hat{T}_{F_2}(1,V) = \hat{T}_{F_1 - F_2}(1,V) = \hat{T}_{F_3}(1,V) - \hat{T}_{F_4}(1,V) \\ &= \hat{T}^{H_1,H_0}_{f^{[1]}}(V) - \hat{T}^{H_0,H_0}_{f^{[1]}}(V), \ \text{ where } T_F = T_F^{H_1,H_0,H_0}, \\ F_1(x,y,z) &= xf^{[2]}(x,y,z),\ \ F_2(x,y,z) = yf^{[2]}(x,y,z), \\ F_3(x,y,z) &= f^{[1]}(x,z),\ \ F_4(x,y,z) = f^{[1]}(y,z). \end{aligned}$$

The proof is finished now via approximation. From the bounded version of the lemma, we have

$$\begin{aligned} E_{1,n}\hat{T}^{H_{1,n},H_{0,n}}_{f^{[1]}}(E_{0,n}VE_{0,n}) - E_{1,n}\hat{T}^{H_{0,n},H_{0,n}}_{f^{[1]}}(E_{0,n}VE_{0,n}) \\ = E_{1,n}T^{H_{1,n},H_{0,n},H_{0,n}}_{f^{[2]}}(H_{1,n} - H_{0,n}, E_{0,n}VE_{0,n}). \end{aligned}$$

By the definition of the transformations T_ϕ and $\hat{T}_\phi$ and algebraic properties of operator integrals, this implies

$$E_{1,n}\hat{T}^{H_1,H_0}_{f^{[1]}}(E_{0,n}VE_{0,n}) - E_{1,n}\hat{T}^{H_0,H_0}_{f^{[1]}}(E_{0,n}VE_{0,n}) = E_{1,n}T^{H_1,H_0,H_0}_{f^{[2]}}(H_1 - H_0, E_{0,n}VE_{0,n}).$$

Observe now that the left hand side converges in the L_2-norm to

$$\hat{T}^{H_1,H_0}_{f^{[1]}}(V) - \hat{T}^{H_0,H_0}_{f^{[1]}}(V)$$

and the right hand side converges in the L_1-norm to

$$T^{H_1,H_0,H_0}_{f^{[2]}}(H_1 - H_0, V)$$

[1] We assume that the intersection of the domains of H_0 and H_1 is dense in $\mathcal{H}$ and denote by $H_1 - H_0$ the closure of the respective algebraic sum.

by Lemma 2.8 and Proposition 2.7. The proof follows. □

Proof. [Proof of Lemma 2.18] It follows from Lemmas 2.15 and 2.19 that

$$\frac{f(H_0+tV)-f(H_0)}{t} - \hat{T}^{H_0,H_0}_{f^{[1]}g^{-1}}(Vg(H_0)) = tT^{H_0+tV,H_0,H_0}_{f^{[2]}g^{-1}}(V,Vg(H_0)),$$

which, clearly, implies

$$\left\|\frac{f(H_0+tV)-f(H_0)}{t} - \hat{T}^{H_0,H_0}_{f^{[1]}g^{-1}}(Vg(H_0))\right\|_1 = O(t), \text{ as } t\to 0. \quad \square$$

LEMMA 2.20. *Let $H_0 = H_0^*$ be affiliated with $\mathcal{M}$ and $V = V^* \in L_2$, let $f \in C_b^2(\mathbb{R})$. If $f \in \mathfrak{C}^2$, then*

$$f(H_0+V) - f(H_0) - \frac{d}{dt}\left[f(H_0+tV)\right]\Big|_{t=0} = T^{H_0+V,H_0,H_0}_{f^{[2]}}(V,V) \in L_1.$$

Proof. The proof is a straightforward corollary of Lemmas 2.15, 2.19, and 2.18 applied with the weight $g \equiv 1$. □

2.4. Double operator integrals under a trace

The representations for traces of double operator integrals derived in this subsection will be used to establish the absolute continuity of Koplienko's SSF.

LEMMA 2.21. ([20, Lemma 8]) *Let $H_0 = H_0^*$ be affiliated with $\mathcal{M}$ and $V = V^* \in L_2$. If Ω is an invertible continuous function and $f \in \mathfrak{C}^1$, then $f^{[1]} \circ \Omega \in \mathfrak{C}^1$ and*

$$T^{H,H_0}_{f^{[1]}\circ\Omega}(V) = T^{\Omega(H),\Omega(H_0)}_{f^{[1]}}(V),$$

where $(f^{[1]}\circ\Omega)(x,y) := f^{[1]}(\Omega(x),\Omega(y))$.

HYPOTHESIS 2.22. *(i) Let $g \in C_0^2(\mathbb{R})$ and let ω be a strictly positive integrable function in $C_0(\mathbb{R})$. Assume, in addition, that $(g^{-2})' \in L_\infty(\mathbb{R})$ and $\omega \in L_\infty(\mathbb{R}, g^{-2}dt)$. Denote*

$$\Omega(\lambda) := \int_{-\infty}^{\lambda} \omega(t)\,dt.$$

(ii) Let $g \in C_0^2(\mathbb{R})$, with $(g^{-1})' \in L_\infty(\mathbb{R})$.

EXAMPLE 2.23. The functions $g(t) = (1+t^2)^{-1/4}$ and $\omega(t) = (1+t^2)^{-1/2-\varepsilon}$, with $\varepsilon > 0$, satisfy Hypothesis 2.22 (i) and $g(t) = (1+t^2)^{-1/2}$ satisfies Hypothesis 2.22 (ii).

THEOREM 2.24. *Let $H = H^*, H_0 = H_0^*$ be affiliated with $\mathcal{M}$ and $V = V^*, W = W^* \in L_2$. Assume Hypothesis 2.22 (i).*

(i) There is a unique finite measure $\xi := \xi_{H,H_0,V,W,\omega,g}$ on $\mathbb{R}$ such that

$$\tau\left(\hat{T}^{H,H_0}_{f^{[1]}}(V)W\right) = \int_{\mathbb{R}} f'(t)\,d\xi(t), \quad \textit{for } f \in C_b^1(\mathbb{R}), \quad \textit{with } f' \in C_0(\mathbb{R}),$$

and

$$\int_{\mathbb{R}} \omega(t)\,d|\xi(t)| \leqslant \left\|\Omega^{[1]}g^{-2}\right\|_\infty \|g(H_0)V\|_2 \, \|g(H_0)W\|_2 .$$

(ii) The mapping $(V,W) \mapsto \xi_{H,H_0,V,W,\omega,g}$ is locally uniformly continuous; for $V_j, W_j \in L_2,\ j = 1,2,$

$$\int_{\mathbb{R}} \omega(t)\,d|\xi_{H,H_0,V_1,W_1,\omega,g}(t) - \xi_{H,H_0,V_2,W_2,\omega,g}(t)|$$
$$\leqslant C_{\omega,g} \max\{\|g(H_0)V_1\|_2, \|g(H_0)W_1\|_2\} \max\{\|g(H_0)(V_1 - V_2)\|_2, \|g(H_0)(W_1 - W_2)\|_2\}.$$

Proof. (i) Let $f \in C_c^2(\mathbb{R})$. It is easy to see that $(f \circ \Omega)^{[1]} = (f^{[1]} \circ \Omega) \cdot \Omega^{[1]}$. By the multiplicativity of the double operator integral (see, e.g., [2, Proposition 4.10 (ii)] or [19, Lemma 3.2]) and by Lemma 2.21,

$$\hat{T}^{H,H_0}_{(f\circ\Omega)^{[1]}}(V) = \hat{T}^{\Omega(H),\Omega(H_0)}_{f^{[1]}}\left(\hat{T}^{H,H_0}_{\Omega^{[1]}}(V)\right).$$

Therefore, substituting f with $f \circ \Omega_{inv}$, and applying Lemma 2.13 (adjusting the reasoning in Lemma 2.16), we derive

$$\hat{T}^{H,H_0}_{f^{[1]}}(V)W = \hat{T}^{\Omega(H),\Omega(H_0)}_{(f\circ\Omega_{inv})^{[1]}}\left(\hat{T}^{H,H_0}_{\Omega^{[1]}}(V)\right)W = \hat{T}^{\Omega(H),\Omega(H_0)}_{(f\circ\Omega_{inv})^{[1]}}\left(\hat{T}^{H,H_0}_{\Omega^{[1]}g^{-2}}(Vg(H_0))\right)(g(H_0)W).$$

(Note that $(f \circ \Omega_{inv})' \in L_\infty(\Omega(\mathbb{R}))$ because f' is compactly supported). From the estimate (2.5), we have

$$\left|\tau\left(\hat{T}^{H,H_0}_{f^{[1]}}(V)W\right)\right| \leqslant \left\|(f \circ \Omega_{inv})'\right\|_{L_\infty(\Omega(\mathbb{R}))} \left\|\Omega^{[1]}g^{-2}\right\|_\infty \|g(H_0)V\|_2 \, \|g(H_0)W\|_2 .$$

Thus, from the Riesz representation theorem for a bounded linear functional on the space of continuous functions on a compact, it follows that there is a unique finite measure $\tilde{\xi}$ such that

$$\tau\left(\hat{T}^{H,H_0}_{f^{[1]}}(V)W\right) = \int_{\Omega(\mathbb{R})} (f \circ \Omega_{inv})'(t)\,d\tilde{\xi}(t) = \int_{\mathbb{R}} f'(t)\,d(\tilde{\xi} \circ \Omega)(t), \quad \text{for } f \in C_c^2(\mathbb{R}),$$

and

$$\int_{\mathbb{R}} \omega(t)\,d|(\tilde{\xi} \circ \Omega)(t)| = \int_{\Omega(\mathbb{R})} d|\tilde{\xi}(t)| \leqslant \left\|\Omega^{[1]}g^{-2}\right\|_\infty \|g(H_0)V\|_2 \, \|g(H_0)W\|_2 .$$

Setting $\xi := \tilde{\xi} \circ \Omega$ proves (i) for $f \in C_c^2(\mathbb{R})$.

Now let $f \in C_b^1(\mathbb{R})$, with $f' \in C_0(\mathbb{R})$. Let $\{f_n\}_{n=1}^\infty \subseteq C_c^2(\mathbb{R})$ be such that $\{f_n'\}_1^\infty$ approximates f' in the supremum norm. Application of Lemma 2.8 (iii) completes the proof of (i).

The claim (ii) can be proved similarly to (i). □

THEOREM 2.25. *Let $H_0 = H_0^*$ and $H = H^*$ be affiliated with $\mathscr{M}$ and $V = V^* \in \mathscr{M}$ be such that $Vg(H_0), Vg(H) \in \mathscr{L}_2$. Assume Hypothesis 2.22 (ii).*

(i) There is a unique locally finite measure $\xi := \xi_{H_0,V,\omega,g}$ such that

$$\tau\left(T_{f^{[1]}}^{H,H_0}(V)V\right) = \int_{\mathbb{R}} f'(t)\, d\xi(t), \quad \text{for } f \in C_c^2(\mathbb{R}),$$

and

$$\int_{[a,b]} d|\xi| \leqslant C_{g,b-a} \|g(H_0)V\|_2 \|g(H)V\|_2 .$$

(ii) For $V_1, V_2 \in \mathscr{L}_2$,

$$\int_{[a,b]} d|\xi_{H,H_0,V_1,\omega,g} - \xi_{H,H_0,V_2,\omega,g}|$$
$$\leqslant C_{g,b-a} \max\{\|g(H_0)V_2\|_2, \|g(H)V_1\|_2\} \max\{\|g(H_0)(V_1-V_2)\|_2, \|g(H)(V_1-V_2)\|_2\}.$$

Proof. Let $f \in C_c^2((a,b))$ (the set of C^2-functions whose closed supports are compact subsets of (a,b)) and let

$$F(x,y) := g^{-1}(x) f^{[1]}(x,y) g^{-1}(y).$$

We will show that $F \in L_\infty(\mathbb{R}^2)$. By applying the Leibnitz formula (2.4) twice, we derive

$$\begin{aligned} F(x,y) &= g^{-1}(x)\left((fg^{-1})^{[1]}(x,y) - f(x)\left(g^{-1}\right)^{[1]}(x,y)\right) \\ &= g^{-1}(x)\left(fg^{-1}\right)^{[1]}(x,y) - g^{-1}(x)f(x)\left(g^{-1}\right)^{[1]}(x,y) \\ &= \left(g^{-1}fg^{-1}\right)^{[1]}(x,y) - \left(g^{-1}\right)^{[1]}(x,y)f(y)g^{-1}(y) - g^{-1}(x)f(x)\left(g^{-1}\right)^{[1]}(x,y). \end{aligned} \tag{2.12}$$

Using the estimate (2.3) and the fact that f is supported in (a,b), we obtain

$$\begin{aligned} \left\|(g^{-1}fg^{-1})^{[1]}\right\|_\infty &\leqslant \|(g^{-1}fg^{-1})'\|_\infty \leqslant 2\|fg^{-1}(g^{-1})'\|_\infty + \|f'g^{-2}\|_\infty \\ &\leqslant \|f\|_\infty \|(g^{-1})'\|_\infty \|g^{-1}\|_{L_\infty([a,b])} + \|f'\|_\infty \|g^{-1}\|_{L_\infty([a,b])}^2 \end{aligned} \tag{2.13}$$

and

$$\left\|\left(g^{-1}\right)^{[1]} fg^{-1}\right\|_\infty \leqslant \|f\|_\infty \|(g^{-1})'\|_\infty \|g^{-1}\|_{L_\infty([a,b])}. \tag{2.14}$$

We also have

$$\|f\|_\infty \leqslant \|f'\|_\infty (b-a) \tag{2.15}$$

and

$$\|g^{-1}\|_{L_\infty([a,b])} \leqslant \|(g^{-1})'\|_\infty (b-a) + |g^{-1}(a)|. \tag{2.16}$$

Combining (2.12)-(2.16) gives the bound

$$\|F\|_\infty \leqslant C_{g,b-a} \|f'\|_\infty. \tag{2.17}$$

Applying Lemma 2.13 (adjusting the reasoning in Lemma 2.16), we obtain

$$T_{f^{[1]}}^{H,H_0}(V)V = \hat{T}_F^{H,H_0}(g(H)V)g(H_0)V \tag{2.18}$$

along with the estimate

$$\left|\tau\left(T_{f^{[1]}}^{H,H_0}(V)V\right)\right| \leqslant C_{g,b-a} \|f'\|_\infty \|g(H_0)V\|_2 \|g(H)V\|_2, \quad \text{for } f \in C_c^2((a,b)).$$

Application of the Riesz representation theorem completes the proof. □

3. Hilbert-Schmidt compatibility.

Let $\mathscr{A} = H_0 + \mathscr{A}_0$ be an affine space of self-adjoint operators affiliated with $\mathscr{M}$, where H_0 is a self-adjoint operator affiliated with $\mathscr{M}$ and $\mathscr{A}_0$ is a locally convex real topological vector space continuously embeddable in the real Banach space of all self-adjoint operators from $\mathscr{M}$.

DEFINITION 3.1. Let $\mathfrak{F}$ be a subset of continuous functions on $\mathbb{R}$. We say that $(\mathfrak{F}, \mathscr{A})$ is *τ-Hilbert-Schmidt compatible* (briefly, τ-HS-compatible) if, for every $\phi \in \mathfrak{F}$, the map

$$\mathscr{A}_0^2 \ni (V_1, V_2) \mapsto \phi(H_0 + V_1)V_2 \tag{3.1}$$

attains values in $\mathscr{L}_2$ and is $\mathscr{L}_2$-continuous.

Since $X \in \mathscr{L}_2$ if and only if $X^* \in \mathscr{L}_2$ and $\|X\|_{2\cap\infty} = \|X^*\|_{2\cap\infty}$, we also have that the map

$$\mathscr{A}_0^2 \ni (V_1, V_2) \mapsto V_1\phi(H_0 + V_2) = V_1\bar{\phi}(H_0 + V_2)\left(\phi\bar{\phi}^{-1}\right)(H_0 + V_2) \tag{3.2}$$

attains values in $\mathscr{L}_2$ and is $\mathscr{L}_2$-continuous, provided the map in (3.1) attains values in $\mathscr{L}_2$ and is $\mathscr{L}_2$-continuous.

DEFINITION 3.2. We say that $(\mathfrak{F}, \mathscr{A})$ is *τ-Hilbert-Schmidt compatible in the weak sense* if, for every $\phi \in \mathfrak{F}$, the map in (3.1) attains values in $\mathscr{L}_2$.

REMARKS 3.3. (i) If $\mathscr{A}_0 \subset \mathscr{L}_2$, then $(L_\infty(\mathbb{R}) \cap \tilde{B}^1_{\infty,1}, \mathscr{A})$ is τ-HS-compatible. This follows from Lemma 2.14 and the estimate (2.2).

(ii) If $(C_c^\infty(\mathbb{R}), \mathscr{A})$ is τ-HS-compatible and H_0 is bounded with $\sigma(H_0) \subset [a,b]$, then $V = \phi(H_0)V \in \mathscr{L}_2$, where $\phi \in C_c^\infty(\mathbb{R})$ and ϕ equals 1 on $[a,b]$. Therefore, the concept of the τ-HS-compatibility is non-trivial only for unbounded operators.

(iii) The above definition of the τ-HS-compatibility is consistent with the definition of the trace class compatibility in [1]. We recall that $\mathscr{A}$ is τ-trace class compatible if for every $f \in C_c^\infty(\mathbb{R})$, the map $\mathscr{A}_0^2 \ni (V_1, V_2) \mapsto f(H_0 + V_1)V_2$ attains values in $\mathscr{L}_1$ and is $\mathscr{L}_1$-continuous. Clearly, for $\mathfrak{F} = C_c^\infty(\mathbb{R})$, τ-trace class compatibility implies τ-HS-compatibility in the sense of Definition 3.1.

Examples of Hilbert-Schmidt compatible operators will be provided in Section 5, and now we establish sufficient conditions for the compatibility.

The Hilbert-Schmidt compatibility for a family of functions can be derived from the HS-compatibility for some simple test function (denoted by g).

THEOREM 3.4. *Let $g \in C_0^2(\mathbb{R})$ be a function without zeros, with $(g^{-1})' \in L_\infty(\mathbb{R})$. If $g(H_0)V \in \mathscr{L}_2$ for any $V \in \mathscr{A}_0$, then $(L_\infty(\mathbb{R}, g^{-1}\,dt), \mathscr{A})$ is τ-HS-compatible in the weak sense. Moreover, for every $\phi \in L_{g^{-1}} \cap L_\infty(\mathbb{R}, g^{-1}\,dt)$,*

$$\sup_{r\in[0,1]} \|\phi(H_0 + rV_1)V_2\|_{2\cap\infty} \leqslant \left\|\phi^{[1]} g^{-1}\right\|_\infty \|g(H_0)V_1\|_{2\cap\infty} \|V_2\|_\infty + \left\|\phi g^{-1}\right\|_\infty \|g(H_0)V_2\|_{2\cap\infty}.$$

Proof. Let $V_1, V_2 \in \mathscr{A}_0$ and $\phi \in L_{g^{-1}} \cap L_\infty(\mathbb{R}, g^{-1}\,dt)$. We have

$$\|\phi(H_0 + V_1)V_2\|_{2\cap\infty} \leqslant \|(\phi(H_0 + V_1) - \phi(H_0))V_2\|_{2\cap\infty} + \|\phi(H_0)V_2\|_{2\cap\infty}.$$

By the inequality $\|AB\|_{2\cap\infty} \leqslant \|A\|_\infty \|B\|_{2\cap\infty}$, for $A \in \mathscr{M}$ and $B \in \mathscr{L}_2$, from Lemma 2.15 and the estimate (2.5), we obtain

$$\left\|\big(\phi(H_0 + V_1) - \phi(H_0)\big)V_2\right\|_{2\cap\infty} \leqslant \|V_2\|_\infty \|\phi^{[1]} g^{-1}\|_\infty \|g(H_0)V_1\|_{2\cap\infty}. \tag{3.3}$$

We also have

$$\|\phi(H_0)V_2\|_{2\cap\infty} = \left\|\phi(H_0)g^{-1}(H_0)g(H_0)V_2\right\|_{2\cap\infty} \leqslant \left\|\phi g^{-1}\right\|_\infty \|g(H_0)V_2\|_{2\cap\infty}.$$

Combining the inequalities above proves $\phi(H_0 + V_1)V_2 \in \mathscr{L}_2$ along with the estimate.

Now let $\phi \in L_\infty(\mathbb{R}, g^{-1}\,dt)$. From the proof above we have $g(H_0 + V_1)V_2 \in \mathscr{L}_2$ for every $V_1, V_2 \in \mathscr{A}_0$. Therefore,

$$\phi(H_0 + V_1)V_2 = (\phi g^{-1})(H_0 + V_1)g(H_0 + V_1)V_2 \in \mathscr{L}_2,$$

proving the τ-HS compatibility of $(L_\infty(\mathbb{R}, g^{-1}\,dt), \mathscr{A})$ in the weak sense, and we have the estimate

$$\|\phi(H_0 + V_1)V_2\|_{2\cap\infty} \leqslant \left\|\phi g^{-1}\right\|_\infty \|g(H_0 + V_1)V_2\|_{2\cap\infty}. \quad \square \tag{3.4}$$

THEOREM 3.5. *Let $g \in C_b(\mathbb{R})$ be a function without zeros. If $(\{g\},\mathscr{A})$ is τ-HS-compatible in the weak sense and $V_2 \mapsto g(H_0+V_1)V_2$ is $\mathscr{L}_2$-continuous locally uniformly with respect to V_1, then $(L_{g^{-1}},\mathscr{A})$ is τ-HS-compatible.*

Proof. Let $\phi \in L_{g^{-1}}$ and let $V_1, V_1', V_2, V_2' \in \mathscr{A}_0$, with (V_1', V_2') close enough to (V_1, V_2) (in the topology of $\mathscr{A}_0^2$). By trivial algebra, we have

$$\begin{aligned}&\left\|\phi(H_0+V_1)V_2-\phi(H_0+V_1')V_2'\right\|_{2\cap\infty}\\&\quad\leqslant\left\|\big(\phi(H_0+V_1)-\phi(H_0+V_1')\big)V_2\right\|_{2\cap\infty}+\left\|\phi(H_0+V_1')(V_2-V_2')\right\|_{2\cap\infty}.\end{aligned}$$

The second summand can be handled with the aid of (3.4) and the assumption on $(\{g\},\mathscr{A})$. For the first summand we have

$$\left\|\big(\phi(H_0+V_1)-\phi(H_0+V_1')\big)V_2\right\|_{2\cap\infty}\leqslant\|\phi(H_0+V_1)-\phi(H_0+V_1')\|_{2\cap\infty}\|V_2\|_\infty.$$

Applying (3.3) guarantees

$$\left\|\big(\phi(H_0+V_1)-\phi(H_0+V_1')\big)V_2\right\|_{2\cap\infty}\leqslant\|V_2\|_\infty\|\phi^{[1]}g^{-1}\|_\infty\|g(H_0+V_1)(V_1-V_1')\|_{2\cap\infty}.$$

Applying the local uniform continuity of $V_2 \mapsto g(H_0+V_1)V_2$ with respect to V_1 completes the proof of the theorem. □

For trace formulae, we need continuity of the map $r \mapsto (f(H_r)-f(H_0))V$ in the $\mathscr{L}_1$-norm, which is proved below under assumptions of the τ-HS-compatibility in the weak sense.

Throughout what follows, H_r denotes the operator H_0+rV, where $V \in \mathscr{A}_0$ and $r \in [0,1]$. Let $\mathfrak{F}$ denote a family of functions in $C^2(\mathbb{R})$.

THEOREM 3.6. *If there is $g \in C_b(\mathbb{R})$ without zeros such that $Vg(H_0) \in \mathscr{L}_2$, then for every $f \in L_{g^{-2}}$, the map*

$$[0,1] \ni r \mapsto \big(f(H_r)-f(H_0)\big)V$$

attains values in $\mathscr{L}_1$ and is $\mathscr{L}_1$-continuous.

Proof. Continuity of the map $r \mapsto \big(f(H_r)-f(H_0)\big)V$ in the operator norm follows from Proposition 2.5 and the estimate (2.2). It follows from Lemma 2.16 that

$$\begin{aligned}\big(f(H_r)-f(H_0)\big)V-\big(f(H_{r_0})-f(H_0)\big)V&=\big(f(H_r)-f(H_{r_0})\big)V\\&=\hat{T}^{H_r,H_{r_0}}_{f^{[1]}g^{-2}}\big((r-r_0)Vg(H_{r_0})\big)\big(g(H_{r_0})V\big).\end{aligned}$$

Applying the estimate (2.5) for a double operator integral on L_2 provides

$$\begin{aligned}&\lim_{r\mapsto r_0}\left\|\big(f(H_r)-f(H_0)\big)V-\big(f(H_{r_0})-f(H_0)\big)V\right\|_1\\&\quad\leqslant\lim_{r\mapsto r_0}\left\|f^{[1]}g^{-2}\right\|_\infty|r-r_0|\left\|Vg(H_{r_0})\right\|_2\left\|g(H_{r_0})V\right\|_2.\end{aligned}$$

Since $\sup_{r\in[0,1]}\|g(H_r)V\|_2<\infty$ by Theorem 3.4, the function $r\mapsto\big(f(H_r)-f(H_0)\big)V$ is L_1-continuous. □

In light of Lemma 2.10, Theorem 3.6 applies to $f\in C_c^2(\mathbb{R})\cup\mathfrak{R}_b$ and $g(t)=(1+t^s)^\alpha$, where $\alpha\in[-\frac{1}{2s},0)$, $s\in 2\mathbb{N}$. As it is shown below, the same class of functions f works for $g(t)=(1+t^s)^\alpha$, with $\alpha\in[-\frac{1}{s},0)$.

THEOREM 3.7. *Let $g(t)=(1+t^s)^\alpha$, where $\alpha\in[-\frac{1}{s},0)$, $s\in 2\mathbb{N}$. If $V\in\mathscr{M}$ is such that $Vg(H_0)\in\mathscr{L}_2$, then for every $f\in C_c^2(\mathbb{R})\cup\mathfrak{R}_b$, the map*

$$[0,1]\ni r\mapsto\big(f(H_r)-f(H_0)\big)V$$

attains values in $\mathscr{L}_1$ and is $\mathscr{L}_1$-continuous.

Proof. Continuity of $r\mapsto\big(f(H_r)-f(H_0)\big)V$ in the operator norm follows from Lemma 2.14.

When $f\in\mathfrak{R}_b$, the result follows from the decomposition (2.7) and properties of the resolvent.

In case $f\in C_c^2(\mathbb{R})$, it is enough to prove the result for $f\geqslant 0$. Indeed, If Ω is an open interval in $\mathbb{R}$ and if $f\in C_c^2(\Omega)$ is real-valued, then there exist functions $f_1,f_2\in C_c^2(\Omega)$ such that f_1 and f_2 are non-negative and $f=f_1-f_2$. We can also make $\sqrt{f_1},\sqrt{f_2}\in C_c^2(\Omega)$.

Note that $f^{[1]}(\lambda_0,\lambda_1)=\frac{\big(\sqrt{f}(\lambda_0)-\sqrt{f}(\lambda_1)\big)\big(\sqrt{f}(\lambda_0)+\sqrt{f}(\lambda_1)\big)}{\lambda_0-\lambda_1}$. Application of Lemmas 2.14 and 2.9 then gives

$$\begin{aligned}f(H_r)-f(H_{r_0})&=T^{H_r,H_{r_0}}_{f^{[1]}}((r-r_0)V)\\&=T^{H_r,H_{r_0}}_{\sqrt{f}^{[1]}}\Big((r-r_0)\sqrt{f}(H_r)V\Big)+T^{H_r,H_{r_0}}_{\sqrt{f}^{[1]}}\Big((r-r_0)V\sqrt{f}(H_{r_0})\Big).\end{aligned}\tag{3.5}$$

(The details of the proof of (3.5) can be found in [3, Lemmas 1.14 and 1.17].) By Lemmas 2.13 and 2.9, for any $U\in\mathscr{L}_2$,

$$T^{H_0+V,H_0}_{\sqrt{f}^{[1]}}(U)V=\hat{T}^{H_0+V,H_0}_{\sqrt{f}^{[1]}g^{-1}}(Ug(H_0))V=\hat{T}^{H_0+V,H_0}_{\sqrt{f}^{[1]}g^{-1}}(U)g(H_0)V,\tag{3.6}$$

where, by the estimate (2.5) and Lemma 2.10,

$$\left\|T^{H_0+V,H_0}_{\sqrt{f}^{[1]}}(U)V\right\|_1\leqslant\left\|\sqrt{f}^{[1]}g^{-1}\right\|_\infty\|U\|_2\,\|g(H_0)V\|_2.\tag{3.7}$$

Applying (3.6) and (3.7) to each summand in (3.5) (with $U=(r-r_0)\sqrt{f}(H_r)V$ and $U=(r-r_0)V\sqrt{f}(H_{r_0})$, respectively) provides

$$\begin{aligned}&\big\|\big(f(H_r)-f(H_{r_0})\big)V\big\|_1\\&\quad\leqslant\left\|\sqrt{f}^{[1]}g^{-1}\right\|_\infty|r-r_0|\left(\left\|\sqrt{f}(H_r)V\right\|_2+\left\|V\sqrt{f}(H_{r_0})\right\|_2\right)\|g(H_{r_0})V\|_2.\end{aligned}\tag{3.8}$$

To complete the proof, we apply the estimate from Theorem 3.4 to $\|\sqrt{f}(H_r)V\|_2$, $\|V\sqrt{f}(H_{r_0})\|_2$, and $\|g(H_{r_0})V\|_2$. □

4. Koplienko's spectral shift function

4.1. Hilbert-Schmidt perturbations

In this subsection, $H_0 = H_0^*$ is defined in $\mathscr{H}$ and $V = V^* \in \mathscr{B}(\mathscr{H})$.

In case when $\mathscr{M} = \mathscr{B}(\mathscr{H})$ and $V \in \mathscr{L}_2$, Koplienko's SSF associated with the pair (H_0,V) is an L_1-function η satisfying

$$\tau\left[f(H_0+V)-f(H_0)-\frac{d}{dr}f(H_0+rV)\bigg|_{r=0}\right]=\int_{\mathbb{R}}f''(t)\eta(t)\,dt, \tag{4.1}$$

for $f \in \mathfrak{R}_b$ [9]. The trace formula (4.1) was extended to $f \in \tilde{B}^2_{\infty,1} \cap \Lambda_1$ in [14]. (If one modifies the left hand side of (4.1), then this formula can be extended to $f \in \tilde{B}^2_{\infty,1}$). Koplienko's SSF in the von Neumann algebra setting is discussed in [8, 19, 25]. It is known that $\eta \geqslant 0$ and $\|\eta\|_1 = \tau(V^2)/2$. When $V \in \mathscr{L}_1$, Koplienko's SSF η can be expressed via Krein's SSF ξ by the formula

$$\eta(t) = -\int_{-\infty}^{t}\xi(\lambda)\,d\lambda + \tau[E_{H_0}((-\infty,t))V]. \tag{4.2}$$

In case when $\mathscr{M} = \mathscr{B}(\mathscr{H})$ and H_0 and V are so that $Vg(H_0) \in \mathscr{L}_2$, with $g(t) = (1+t^2)^{-1/4}$, Koplienko proved existence of the function η integrable with weight $(1+t^2)^{-1/2-\varepsilon}$, $\varepsilon > 0$, and satisfying the trace formula (4.1) for $f \in \mathfrak{R}_b$. The trace formula (4.1) was also derived in [5] for pseudo-differential operators.

We will need the following spectral averaging formulae.

LEMMA 4.1. *Let $H_0 = H_0^*$ be affiliated with $\mathscr{M}$, and $V \in \mathscr{L}_2$, let $f \in \tilde{B}^2_{\infty,1} \cap \tilde{B}^1_{\infty,1}$. If $f' \in \tilde{B}^1_{\infty,1}$, then*

$$\tau\left(f(H_0+V)-f(H_0)-\frac{d}{dr}f(H_0+rV)\bigg|_{r=0}\right)=\int_0^1\tau\Big(\big(f'(H_0+rV)-f'(H_0)\big)V\Big)\,dr.$$

Proof. By [22, Theorem 1.43, Corollary 1.45] and L_1-continuity of the derivative $r \mapsto \frac{d^2}{dr^2}\big(f(H_r)-f(H_0)\big)$ (following from Proposition 2.17 and Lemma 2.8),

$$\tau\left[f(H_0+V)-f(H_0)-\frac{d}{dr}f(H_r)\bigg|_{r=0}\right]=2\int_0^1(1-r)\tau\left[\frac{d^2}{dr^2}\big(f(H_r)-f(H_0)\big)\right]dr. \tag{4.3}$$

We have

$$\begin{aligned}\tau\left[\frac{d^2}{dr^2}\big(f(H_r)-f(H_0)\big)\right] &= \tau\left[\frac{d}{dr}\big(f'(H_r)V-f'(H_0)V\big)\right]\\ &= \frac{d}{dr}\tau\left[\big(f'(H_r)V-f'(H_0)V\big)\right]\end{aligned}$$

(see, e.g., [24, Corollary 3.15] for details). Since $f' \in \tilde{B}^1_{\infty,1}$, from Proposition 2.6, $(f')^{[1]} \in \mathfrak{C}^1$. Thus, we also have $\big(f'(H_r)V - f'(H_0)V\big) \in \mathscr{L}_1$ by Lemma 2.14. Integrating by parts in (4.3) implies

$$\tau\left[f(H_0+V) - f(H_0) - \frac{d}{dr}f(H_r)\bigg|_{r=0}\right] = \int_0^1 \tau[(f'(H_r) - f'(H_0))V]\,dr. \quad \square$$

LEMMA 4.2. *For $V \in \mathscr{L}_2$ and $f \in L_\infty(\mathbb{R}) \cap \tilde{B}^1_{\infty,1}$, with $f' \in C_0(\mathbb{R})$,*

$$\int_0^1 \tau[(f(H_0+rV) - f(H_0))V]\,dr = \int_{\mathbb{R}} f'(t)\eta(t)\,dt. \tag{4.4}$$

Proof. For $V \in \mathscr{L}_1$ and $f \in L_\infty(\mathbb{R}) \cap \tilde{B}^1_{\infty,1}$, the representation (4.4) with η given by (4.2) can be derived from [9] with application of the Birman-Solomyak spectral averaging representation for ξ.

For $V \in \mathscr{L}_2$ and f a derivative of a function from Lemma 4.1, the representation (4.4) is a consequence of Lemma 4.1 and the representation (4.1).

The general case follows via approximation as in the proof of Theorem 2.24. $\square$

In case $V \in \mathscr{L}_2$, the left-hand side of (4.4) is bounded by $\|f'\|_\infty \|V\|_2^2$ (use Lemma 2.14 and (2.5)) and, therefore, defines a bounded functional on the functions f'. Moreover, the left-hand side of (4.4) is well defined in case of HS-compatible perturbations and the respective functional possesses properties similar to those of Koplienko's SSF. The generalized Koplienko's SSF for the Hilbert-Schmidt compatible perturbations is discussed below.

4.2. Hilbert-Schmidt compatible perturbations

DEFINITION 4.3. Let $H_0 = H_0^*$ be affiliated with $\mathscr{M}$ and $V = V^* \in \mathscr{M}$. Let g be a function in $C_b(\mathbb{R})$ without zeros. Assume that $g(H_0)V \in \mathscr{L}_2$. We define a generalized Koplienko's SSF to be the functional

$$\Xi(f') := \int_0^1 \tau[(f(H_0+rV) - f(H_0))V]\,dr, \tag{4.5}$$

for $f \in L_{g^{-2}}$.

REMARK 4.4. The functional in (4.5) is well defined in view of Theorem 3.6 (see also Theorem 3.7).

In the series of propositions below, we prove that if we have a compatibility condition with $(g^{-1})' \in L_\infty(\mathbb{R})$, then the functional Ξ is given by a locally finite positive measure. More information about this measure is derived under some additional assumptions.

In the first series of results, we also assume that $(g^{-2})' \in L_\infty(\mathbb{R})$.

THEOREM 4.5. *Let $H_0 = H_0^*$ be affiliated with $\mathscr{M}$ and $V = V^* \in \mathscr{M}$. Assume Hypothesis 2.22 (i) and assume that $Vg(H_0) \in \mathscr{L}_2$. Then, there is a non-negative function $\eta := \eta_{H_0,V,\omega,g} \in L_1(\mathbb{R}, \omega\, dt)$ such that*

$$\Xi(f') = \int_{\mathbb{R}} f'(t)\eta(t)\,dt, \quad \text{for } f \in \mathfrak{C}^1_{g^{-2}}, \text{ with } f' \in L_\infty(\mathbb{R}, \omega^{-1}dt), \tag{4.6}$$

and

$$\int_{\mathbb{R}} |\eta(t)|\,\omega(t)\,dt \leqslant \left\|\Omega^{[1]} g^{-2}\right\|_\infty \|Vg(H_0)\|_2^2.$$

Proof. Let $E_n := E_{H_0}((-n,n))$, $V_n := E_n V E_n$, and $H_{n,r} := H_0 + rV_n$. It is straightforward to see that

$$\|V_n g(H_0)\|_2 \leqslant \|Vg(H_0)\|_2 \quad \text{and} \quad \lim_{n,m\to\infty} \|V_n g(H_0) - V_m g(H_0)\|_2 = 0.$$

Let $\xi_{n,r} := \xi_{H_{n,r},H_0,V_n,V_n,g}$ and $\tilde{\xi}_{n,r}$ be the measures from Theorem 2.24. By Lemma 2.14 and Theorem 2.24, we have

$$\tau\big((f(H_{n,r}) - f(H_0))V_n\big) = \int_{\mathbb{R}} f'(t)\,d\xi_{n,r}(t) = \int_{\Omega(\mathbb{R})} (f \circ \Omega_{inv})'(t)\,d\tilde{\xi}_{n,r}(t), \tag{4.7}$$

for f as in (4.6), and

$$\int_{\mathbb{R}} \omega(t)\,d|\xi_{n,r}(t)| \leqslant \|\Omega^{[1]} g^{-2}\|_\infty \|Vg(H_0)\|_2^2.$$

Since $V_n = \chi_{(-n,n)}(H_0) V \chi_{(-n,n)}(H_0) \in \mathscr{L}_2$ (in view of Theorem 3.4), by the previous subsection and Lemma 4.2, there is a unique non-negative L_1-function η_n satisfying

$$\int_0^1 \tau\big((f(H_{n,r}) - f(H_0))V_n\big)\,dr = \int_{\mathbb{R}} f'(t)\eta_n(t)\,dt,$$
$$\text{for } f \in L_\infty(\mathbb{R}) \cap \tilde{B}^1_{\infty,1}, \text{ with } f' \in C_0(\mathbb{R}). \tag{4.8}$$

Upon comparing (4.7) and (4.8), we derive

$$\int_{\mathbb{R}} |\eta_n(t)|\,\omega(t)\,dt \leqslant \|\Omega^{[1]} g^{-2}\|_\infty \|Vg(H_0)\|_2^2.$$

Lemma 2.14 ensures

$$\begin{aligned} &\big(f(H_{n,r}) - f(H_0)\big)V_n - \big(f(H_{m,r}) - f(H_0)\big)V_m \\ &\quad = \big(f(H_{n,r}) - f(H_{m,r})\big)V_n + \big(f(H_{m,r}) - f(H_0)\big)(V_n - V_m) \\ &\quad = T_{f^{[1]}}^{H_{n,r},H_{m,r}}(r(V_n - V_m))V_n + T_{f^{[1]}}^{H_{m,r},H_0}(rV_m)(V_n - V_m). \end{aligned} \tag{4.9}$$

Integrating with respect to r in (4.9), we obtain

$$\begin{aligned} &\int_{\Omega(\mathbb{R})} (f \circ \Omega_{inv})'(t)\,d(\tilde{\xi}_{n,r} - \tilde{\xi}_{m,r})(t) \\ &\quad = \int_{\Omega(\mathbb{R})} (f \circ \Omega_{inv})'(t)\,d\big(\tilde{\xi}_{H_{n,r},H_{m,r},r(V_n-V_m),V_n} + \tilde{\xi}_{H_{m,r},H_0,rV_m,V_n-V_m}\big)(t). \end{aligned}$$

As in the proof of Theorem 2.24 (i), we derive

$$\begin{aligned}&\left|\int_{\Omega(\mathbb{R})}(f\circ\Omega_{inv})'(t)\,d(\tilde{\xi}_{n,r}-\tilde{\xi}_{m,r})(t)\right|\\&\qquad\leqslant 2\left\|(f\circ\Omega_{inv})'\right\|_{L_\infty(\Omega(\mathbb{R}))}\left\|\Omega^{[1]}g^{-2}\right\|_\infty\|Vg(H_0)\|_2\,\|(V_n-V_m)g(H_0)\|_2\,,\end{aligned}$$

which implies

$$\int_{\mathbb{R}}\omega(t)\,d\,|(\xi_{n,r}-\xi_{m,r})(t)|\leqslant C_{\omega,g}\,\|Vg(H_0)\|_2\,\|(V_n-V_m)g(H_0)\|_2\,.$$

Therefore,

$$\int_{\mathbb{R}}|\eta_n(t)-\eta_m(t)|\,\omega(t)\,dt\leqslant C_{\omega,g}\,\|Vg(H_0)\|_2\,\|(V_n-V_m)g(H_0)\|_2\,,$$

that is, the sequence $\{\eta_n\}_{n\geqslant 1}$ converges in $L_1(\mathbb{R},\omega dt)$. Lemma 2.16 implies

$$\begin{aligned}(f(H_r)-f(H_0))V&=T^{H_r,H_0}_{f^{[1]}g^{-2}}(rVg(H_0))(g(H_0)V),\\(f(H_{n,r})-f(H_0))V_n&=T^{H_{n,r},H_0}_{f^{[1]}g^{-2}}(rV_ng(H_0))(g(H_0)V_n).\end{aligned}\tag{4.10}$$

The sequence $\{H_{n,r}\}_n$ converges to H_r in the strong resolvent sense for every r. Therefore, the double operator integrals on the right hand side of (4.10) converge (by Lemma 2.8 (i) and (ii)), which implies convergence of the sequence $\{(f(H_{n,r})-f(H_0))V_n\}_n$ to $(f(H_r)-f(H_0))V$ in L_1. Moreover, the family $\{(f(H_{n,r})-f(H_0))V_n\}_{n,r}$ is uniformly bounded in the L_1-norm and, hence, the left hand side in (4.8) converges to $\int_0^1\tau\left[(f(H_r)-f(H_0))V\right]dr$. Letting $\eta:=\lim_{n\to\infty}\eta_n$ completes the proof of the theorem. □

More specific description of functions satisfying the trace formula (4.6) is given in the corollary below.

COROLLARY 4.6. *Assume the hypothesis of Theorem 4.5. Assume, in addition, that* $g(t)=(1+t^s)^\alpha$, *where* $\alpha\in\left[-\frac{1}{2s},0\right)$, $s\in 2\mathbb{N}$, *and* H_0 *is bounded from below. Then, for every* f *as in Lemma 2.12,*

$$\Xi(f')=\int_{\mathbb{R}}f'(t)\eta(t)\,dt.$$

Proof. It is enough to prove the result only in the case $H_r\geqslant\delta I$ for $\delta>0$, with $r\in[0,1]$, and then apply it to the translated operators $H_r+(\delta-a)I$, where $H_r\geqslant aI$ (and to the translated functions $f\circ(t\mapsto t-(\delta-a))$).

Assume that $H_r\geqslant\delta I$, with $\delta>0$. Lemma 2.14 implies

$$(f(H_r)-f(H_0))V=T^{H_r,H_0}_{f^{[1]}}(rV)V=T^{H_r,H_0}_{\phi_{1,\delta}}(rV)V,$$

where
$$\phi_{1,\delta}(\lambda_0,\lambda_1)=f^{[1]}(\lambda_0,\lambda_1)\psi_\delta(\lambda_0)\psi_\delta(\lambda_1),$$
with ψ_δ as in Lemma 2.12. Applying Lemma 2.16 ensures
$$(f(H_r)-f(H_0))V=T^{H_r,H_0}_{\phi_{1,\delta}g^{-2}}(rVg(H_0))(g(H_0)V),$$
where $\phi_{1,\delta}g^{-2}\in\mathfrak{C}^1$ by Lemma 2.12. Similarly,
$$(f(H_{n,r})-f(H_n))V_n=T^{H_{n,r},H_0}_{\phi_{1,\delta}g^{-2}}(rV_ng(H_0))(g(H_0)V_n).$$
Repeating the approximation argument in the proof of Theorem 4.5 completes the proof. □

We also obtain Koplienko's trace formula, which was established in [9] for $g(t)=(1+t^2)^{-\frac{1}{4}}$ under the restriction $f\in\mathfrak{R}_b$.

THEOREM 4.7. *Let $H_0=H_0^*$ be affiliated with $\mathscr{M}$ and $V=V^*\in\mathscr{M}$. Assume Hypothesis 2.22 (i) and assume that $Vg(H_0)\in\mathscr{L}_2$. Then,*
$$\tau\left(f(H_0+V)-f(H_0)-\frac{d}{dr}f(H_0+rV)\bigg|_{r=0}\right)=\int_{\mathbb{R}}f''(t)\eta(t)\,dt,$$
for $f\in L_{g^{-1}}\cap\mathfrak{C}^2_{g^{-2}}\cap\tilde{B}^2_{\infty,1}\cap\tilde{B}^1_{\infty,1}$, with $f''\in L_\infty(\mathbb{R},\omega^{-1}dt)$ and $f'\in\tilde{B}^1_{\infty,1}$.

Proof. Let $E_n:=E_{H_0}((-n,n))$, $V_n:=E_nVE_n$, and $H_{n,r}:=H_0+rV_n$. Let
$$R_2(f,H_0,V_n):=f(H_0+V_n)-f(H_0)-\frac{d}{dr}f(H_0+rV_n)\bigg|_{r=0}.$$
Applying Lemma 4.1 and (4.1) ensures
$$\tau\big(R_2(f,H_0,V_n)\big)=\int_0^1\tau\big((f'(H_{n,r})-f'(H_0))V_n\big)\,dr=\int_{\mathbb{R}}f''(t)\eta_n(t)\,dt.$$
By Lemmas 2.20 and 2.16,
$$R_2(f,H_0,V_n)=T^{H_0+V_n,H_0,H_0}_{f^{[2]}}(V_n,V_n)=T^{H_0+V_n,H_0,H_0}_{f^{[2]}}(V_n,V_n)$$
$$=T^{H_0+V_n,H_0,H_0}_{f^{[2]}g^{-2}}(V_ng(H_0),g(H_0)V_n).$$
Therefore, by continuity of multiple operator integrals (see Lemma 2.8 (i) and (ii), the sequence $\{R_2(f,H_0,V_n)\}_{n\geqslant1}$ converges in L_1. By Lemmas 2.18 and 2.13, we also have
$$R_2(f,H_0,V_n)=f(H_0+V_n)-f(H_0)-E_n\hat{T}^{H_0,H_0}_{f^{[1]}g^{-1}}(Vg(H_0))E_n.$$
The sequence $\{f(H_0+V_n)-f(H_0)\}_{n\geqslant1}$ converges to $f(H_0+V)-f(H_0)$ in the weak

operator topology[2] and $\left\{E_n\hat{T}^{H_0,H_0}_{f^{[1]}g^{-1}}(Vg(H_0))E_n\right\}_{n\geqslant 1}$ converges to $\hat{T}^{H_0,H_0}_{f^{[1]}g^{-1}}(Vg(H_0))$ in the L_2-norm.[3] By Lemma 2.18, the derivative $\frac{d}{dr}f(H_0+rV)\big|_{r=0}=\hat{T}^{H_0,H_0}_{f^{[1]}g^{-1}}(Vg(H_0))$ exists in the $L_1(\mathscr{M},\tau)$-norm, for $f\in L_{g^{-1}}\cap\mathfrak{C}^2_{g^{-1}}$. Consequently, $\{R_2(f,H_0,V_n)\}_{n\geqslant 1}$ converges to $f(H_0+V)-f(H_0)-\frac{d}{dr}f(H_0+rV)\big|_{r=0}$ (in the weak*-topology of the space $L_\infty+L_2$ and also in L_1). Since $\{\eta_n\}_{n\geqslant 1}$ converges to η in $L_1(\mathbb{R},\omega dt)$, the result follows. □

COROLLARY 4.8. *Assume the hypothesis of Theorem 4.7. Assume, in addition, that* $g(t)=(1+t^s)^\alpha$*, where* $\alpha\in\left[-\frac{1}{2s},0\right)$*,* $s\in 2\mathbb{N}$*, and* H_0 *is bounded from below. Then, the trace formula*

$$\tau\left(f(H_0+V)-f(H_0)-\frac{d}{dr}f(H_0+rV)\bigg|_{r=0}\right)=\int_{\mathbb{R}}f''(t)\eta(t)\,dt$$

holds for f *as in Lemma 2.12.*

Proof. Without loss of generality we can assume that $H_r\geqslant\delta I$, for some $\delta>0$. The proof goes similarly to the one of Theorem 4.7, with use of the representation

$$R_2(f,H_0,V_n)=T^{H_0+V_n,H_0,H_0}_{\phi_{2,\delta}g^{-2}}(V_ng(H_0),g(H_0)V_n)$$

and Lemma 2.8. □

A case of a more general compatibility condition with $(g^{-1})'\in L_\infty(\mathbb{R})$ is discussed below.

THEOREM 4.9. *Let* $H_0=H_0^*$ *be affiliated with* $\mathscr{M}$ *and* $V=V^*\in\mathscr{M}$*. Assume Hypothesis 2.22 (ii) and assume that* $Vg(H_0)\in\mathscr{L}_2$*. Then, there is a unique locally finite measure* $\eta:=\eta_{H_0,V,g}$ *such that*

$$\Xi(f')=\int_{\mathbb{R}}f'(t)\,d\eta(t),\quad \textit{for } f\in C_c^2(\mathbb{R}),$$

and

$$\int_{[a,b]}d|\eta(t)|\leqslant C_{g,b-a}\,\|Vg(H_0)\|_2\,\|Vg(H_0+V)\|_2\,.$$

Proof. Since $Vg(H_0)\in\mathscr{L}_2$, Theorem 3.4 implies that $Vg(H_0+V)\in\mathscr{L}_2$ and

$$\|g(H_0+V)V\|_2\leqslant\left\|(g^{-1})'\right\|_\infty\|g\|_\infty\|g(H_0)V\|_{2\cap\infty}\|V\|_\infty+\|g(H_0)V\|_{2\cap\infty}.$$

[2]This follows from Theorems VIII.25.(a) and VIII.20 of [21].

[3]In the case $V\in L_2$, it is enough to use $T^{H_0,H_0}_{f^{[1]}}(V)$ instead of $\hat{T}^{H_0,H_0}_{f^{[1]}g^{-1}}(Vg(H_0))$.

From Lemma 2.14 and Theorem 2.25, we have

$$\sup_{r\in[0,1]} \left|\tau[(f(H_r)-f(H_0))V]\right| = \sup_{r\in[0,1]} \left|\tau[T_{f^{[1]}}^{H_r,H_0}(rV)V]\right| \tag{4.11}$$

$$\leqslant C_{g,b-a}\left\|f'\right\|_\infty \|g(H_0)V\|_2\,\|g(H_0+V)V\|_2\,, \tag{4.12}$$

for f supported in $[a,b]$. The Riesz representation theorem completes the proof. □

THEOREM 4.10. *Assume the hypothesis of Theorem 4.9. Assume, in addition, that* $g(t)=(1+t^s)^\alpha$, *where* $\alpha\in\left[-\frac{1}{s},0\right)$, $s\in 2\mathbb{N}$, *and* H_0 *is bounded from below. Then, the measure* η, *in Theorem 4.9, is absolutely continuous and positive.*

Proof. Let $E_n := E_{H_0}((-n,n))$, $V_n := E_nVE_n$, and $H_{n,r} := H_0+rV_n$. By Lemma 4.2, we have

$$\int_0^1 \tau\big((f(H_{n,r})-f(H_0))V_n\big)\,dr = \int_{\mathbb{R}} f'(t)\eta_n(t)\,dt, \quad \text{for } f\in C_c^2(\mathbb{R}), \tag{4.13}$$

where η_n is a nonnegative function in $L_1(\mathbb{R})$. In (4.9), we derived

$$\big(f(H_{n,r})-f(H_0)\big)V_n-\big(f(H_{m,r})-f(H_0)\big)V_m$$
$$=T_{f^{[1]}}^{H_{n,r},H_{m,r}}(r(V_n-V_m))V_n+T_{f^{[1]}}^{H_{m,r},H_0}(rV_m)(V_n-V_m),$$

which, by (2.18) (from the proof of Theorem 2.25), equals

$$\hat{T}_F^{H_{n,r},H_{m,r}}(rg(H_{n,r})(V_n-V_m))g(H_{m,r})V_n+\hat{T}_F^{H_{m,r},H_0}(rg(H_{m,r})V_m)g(H_0)(V_n-V_m).$$

Along with the estimate of Theorem 3.4 and (2.17), the latter implies

$$\left|\tau\big((f(H_{n,r})-f(H_0))V_n\big)-\tau\big((f(H_{m,r})-f(H_0))V_m\big)\right|$$
$$\leqslant C_{g,b-a,V}\left\|f'\right\|_\infty\big(\|g(H_{n,r})(V_n-V_m)\|_2+\|g(H_0)(V_n-V_m)\|_2\big)\,\|g(H_0)V\|_2\,, \tag{4.14}$$

for $f\in C_c^2((a,b))$. The first summand in (4.14) satisfies the trivial inequality

$$\|g(H_{n,r})(V_n-V_m)\|_2\leqslant\|(g(H_{n,r})-g(H_0))(V_n-V_m)\|_2+\|g(H_0)(V_n-V_m)\|_2\,,$$

in which we need to estimate the first term. Note that $g\in\tilde{B}^1_{\infty,1}$ by Proposition 2.5. Since g satisfies the inequality (2.8) from Lemma 2.12, we also have $\phi_{g,1,\delta}g^{-1}\in\mathfrak{C}^1$, where $\phi_{g,1,\delta}=\phi_{1,\delta}$ is given by (2.9), with $f=g$. Since for the proof it is enough to assume that $H_{n,r}\geqslant\delta I$, for some $\delta>0$, subsequent application of Proposition 2.6, Lemma 2.14, and an analogue of Lemma 2.9 for double operator integrals with symbols in $\mathfrak{C}^1$ gives

$$(g(H_{n,r})-g(H_0))(V_n-V_m)=T_{\phi_{g,1,\delta}g^{-1}}^{H_{n,r},H_0}(rV_n)g(H_0)(V_n-V_m).$$

Thus,

$$\|(g(H_{n,r})-g(H_0))(V_n-V_m)\|_2 \leqslant \left\|\phi_{g,1,\delta}g^{-1}\right\|_{\mathfrak{A}^1} \|V_n\|_\infty \|g(H_0)(V_n-V_m)\|_2$$

and

$$\|g(H_{n,r})(V_n-V_m)\|_2 \leqslant C_{g,V}\,\|g(H_0)(V_n-V_m)\|_2\,. \tag{4.15}$$

Combining (4.14) and (4.15) implies

$$\int_{[a,b]} |\eta_n(t)-\eta_m(t)|\,dt \leqslant C_{g,b-a,V}\,\|g(H_0)V\|_2\,\|g(H_0)(V_n-V_m)\|_2$$

and, hence, convergence of the sequence $\{\eta_n\}_{n\geqslant 1}$ in $L_1^{loc}(\mathbb{R})$.

Similarly,

$$\begin{aligned}&\left|\tau\big((f(H_{n,r})-f(H_0))V_n\big)-\tau\big((f(H_r)-f(H_0))V\big)\right|\\&\quad\leqslant C_{g,b-a,V}\left\|f'\right\|_\infty \|g(H_0)V\|_2\,\|g(H_0)(V_n-V)\|_2\,.\end{aligned}$$

Thus, $\left\{\tau\big((f(H_{n,r})-f(H_0))V_n\big)\right\}_{n\geqslant 1}$ converges to $\tau\big((f(H_r)-f(H_0))V\big)$ uniformly in r and the left hand side of (4.13) converges to $\Xi(f')$. The density of the measure η is the L_1^{loc}-limit of $\{\eta_n\}_{n\geqslant 1}$. □

4.3. Koplienko's SSF for trace-compatible operators

Koplienko's SSF for trace class operators can be expressed in terms of Krein's SSF; likewise, the generalized Koplienko's SSF for trace-compatible operators can be expressed in terms of the generalized Krein's SSF for trace-compatible operators.

We recall that in the case when $\mathscr{A}$ is trace class compatible [1, p. 1771], generalized Krein's spectral shift function ξ is defined as the integral

$$\xi_{H_0,V}(f)=\int_0^1 \tau[f(H_r)V]\,dr, \quad f\in C_c^\infty(\mathbb{R}), \tag{4.16}$$

and satisfies Krein's trace formula [1, Proposition 2.5]

$$\xi_{H_0,V}(f')=\tau\big[f(H_1)-f(H_0)\big], \quad f\in C_c^\infty(\mathbb{R}). \tag{4.17}$$

The requirement $f\in C_c^\infty(\mathbb{R})$ in (4.16) and (4.17) can be relaxed to $f\in C_c^2(\mathbb{R})$.

LEMMA 4.11. *If $\mathscr{A}$ is trace class compatible, then*

$$\Xi(f')=\xi_{H_1,V}(f)-\tau[f(H_0)V], \quad f\in C_c^2(\mathbb{R}).$$

Proof. By the trace class compatibility of $\mathscr{A}$, $r\mapsto f(H_r)V$ is $\mathscr{L}_1$-continuous and, thus,

$$\Xi(f')=\int_0^1 \big(\tau[f(H_r)V]-\tau[f(H_0)V]\big)\,dr,$$

which along with (4.16) completes the proof. □

5. Examples of Hilbert-Schmidt compatible operators

5.1. Fractional powers of the Laplacian.

Let Δ denote the positive scalar Laplacian of $\mathbb{R}^n$ (classical Laplacian multiplied by -1). We set $\mathscr{A} := \Delta^{\frac{n}{4}+\varepsilon} + \mathscr{A}_0$, where $\varepsilon > 0$ and $\mathscr{A}_0 := L_\infty(\mathbb{R}^n)_{s.a.} \cap L_2(\mathbb{R}^n)_{s.a.}$ is endowed with the metric topology associated with the norm $\|.\|_\infty + \|.\|_2$ and acts on $L_2(\mathbb{R}^n)$ by pointwise multiplication operators. We will see below that $\mathscr{A}$ is an affine set of Hilbert-Schmidt compatible operators.

Let $\nabla := (\partial_1, \cdots, \partial_n)$ and $f(t)$ denote the operator of pointwise multiplication by a function f measurable on $\mathbb{R}^n$. Let $f(t)g(-\mathrm{i}\nabla)$ denote a bounded operator A with the inner product

$$\langle x, Ay\rangle = \left\langle \bar{f}x, \mathscr{F}^{-1}(g\mathscr{F}(y))\right\rangle,$$

where $x \in \{h \in L_2(\mathbb{R}^n) : fh \in L_2(\mathbb{R}^n)\}$ and $\mathscr{F}(y) := \widehat{y} \in \{h \in L_2(\mathbb{R}^n) : gh \in L_2(\mathbb{R}^n)\}$. When $f, g \in L_\infty(\mathbb{R}^n)$, we trivially have the bound for the operator norm:

$$\|f(t)g(-\mathrm{i}\nabla)\|_\infty \leqslant \|f\|_\infty \|g\|_\infty.$$

It follows from [23, Theorem 4.1 and Proposition 4.4] that the operator $f(t)g(-\mathrm{i}\nabla)$ is in the Hilbert-Schmidt class if and only if $f, g \in L_2(\mathbb{R}^n)$; moreover,

$$\|f(t)g(-\mathrm{i}\nabla)\|_2 = (2\pi)^{-n/2} \|f\|_2 \|g\|_2. \tag{5.1}$$

By [23, Theorem 4.5 and Proposition 4.7], $f(t)g(-\mathrm{i}\nabla)$ is in the trace class if and only if $f, g \in \ell_1(L_2)$; moreover,

$$\|f(t)g(-\mathrm{i}\nabla)\|_1 \leqslant C \|f\|_{\ell^1(L_2)} \|g\|_{\ell^1(L_2)}.$$

Since $\ell_1(L_2)$ is a proper subspace of $L_1(\mathbb{R}^d) \cap L_2(\mathbb{R}^d)$, there are f and g such that $f(t)g(-\mathrm{i}\nabla) \in \mathscr{L}_2 \setminus \mathscr{L}_1$, where $\mathscr{M} = \mathscr{B}(\mathscr{H})$. Thus, the notions of trace compatibility and HS-compatibility are not equivalent.

LEMMA 5.1. *Let $f \in L_2(\mathbb{R}^n)$. If $\phi \in L_2(\mathbb{R}, t^{\frac{n}{\beta}-1}dt)$, where $\beta \leqslant n$, then $f(t)\phi(\Delta^{\frac{\beta}{2}}) \in \mathscr{L}_2$ and*

$$\left\|f(t)\phi(\Delta^{\frac{\beta}{2}})\right\|_2 = C_{n,\beta} \|f\|_2 \|\phi\|_{L_2(\mathbb{R}, t^{n/\beta-1}dt)}.$$

Proof. Let $g(\vec{x}) := \phi(\|\vec{x}\|^\beta)$ for $\vec{x} \in \mathbb{R}^n$; then, $g(-\mathrm{i}\nabla) = \phi\left(\Delta^{\frac{\beta}{2}}\right)$. By changing to n-dimensional spherical coordinates, one can see that $g \in L_2(\mathbb{R}^n)$ and, thus, the result follows from (5.1). □

Note that the function $g_1(t) = (1+t^s)^{-\frac{1}{2s}}$, $s \in 2\mathbb{N}$, determining a compatibility condition, is not in $L_2(\mathbb{R})$. Nonetheless, we have $\phi = g_1 \circ (t \mapsto t^\gamma) \in L_2(\mathbb{R})$ if $\gamma > 1$ and, hence, by Lemma 5.1, $f(t)g_1(\Delta^{\frac{n\gamma}{2}}) = f(t)\phi(\Delta^{\frac{n}{2}}) \in \mathscr{L}_2$. Therefore, for any $n \in \mathbb{N}$, $\varepsilon > 0$, we have $f(t)g_1(\Delta^{\frac{n}{2}+\varepsilon}) \in \mathscr{L}_2$. More generally, by Theorem 3.4, we have the following lemma.

LEMMA 5.2. *For any* $\varepsilon > 0$,

$$\left(L_\infty(\mathbb{R}, g_1^{-1}dt), \Delta^{\frac{n}{2}+\varepsilon} + \mathscr{A}_0\right) \text{ is weakly HS-compatible,}$$

where $\mathscr{A}_0$ *is a subspace of all multiplication operators by functions from*

$$L_2(\mathbb{R}^n)_{s.a.} \cap L_\infty(\mathbb{R}^n)_{s.a.}$$

Employment of the function $g_2(t) = (1+t^s)^{-\frac{1}{s}}$ allows to verify compatibility for more general operators than in [9]. Indeed, $\phi = g_2 \circ (t \mapsto t^\gamma) \in L_2(\mathbb{R})$ for $\gamma > \frac{1}{2}$ and

$$f(t)g_2(\Delta^{\frac{n}{4}+\varepsilon}) \in \mathscr{L}_2 \quad \text{and} \quad \left\| f(t)g_2(\Delta^{\frac{n}{4}+\varepsilon}) \right\|_2 = \|f\|_2 C_{g_2,n,\varepsilon}, \tag{5.2}$$

for some $C_{g_2,n,\varepsilon} \in \mathbb{R}_+$.

THEOREM 5.3. *For any* $\varepsilon > 0$,

$$\left(L_{g_2^{-1}}, \Delta^{\frac{n}{4}+\varepsilon} + L_2(\mathbb{R}^n)_{s.a.} \cap L_\infty(\mathbb{R}^n)_{s.a.}\right) \text{ is HS-compatible.}$$

Proof. Let V denote an operator of multiplication by a real-valued function f in $L_2(\mathbb{R}^n) \cap L_\infty(\mathbb{R}^n)$. From (5.2) and Theorem 3.4, we derive that the mapping $V_2 \mapsto g_2(\Delta^{\frac{n}{4}+\varepsilon} + V_1)V_2$ is $\mathscr{L}_2$-continuous locally uniformly with respect to V_1. Therefore, application of Theorem 3.5 completes the proof. □

5.2. Perturbation via the Moyal product.

In this example, the vector space $\mathscr{A}_0$ is a noncommutative Hilbert-algebra, based on the Moyal product [7]. The Moyal product of a pair of functions (or distributions) f, g on $\mathbb{R}^{2n}$, is given by

$$f \star_\theta g(x) := (\pi\theta)^{-2n} \iint e^{\frac{2i}{\theta}\omega_0(x-y, x-z)} f(y)g(z)\, d^{2n}y\, d^{2n}z,$$

with $\theta \in \mathbb{R} \setminus \{0\}$ (playing the role of the Planck constant) and ω_0 the canonical symplectic form of $\mathbb{R}^{2n}$. This product is the composition law of symbols associated with the Weyl pseudo-differential calculus on $\mathbb{R}^n$. Since this Weyl map is a unitary operator from the Hilbert space $L_2(\mathbb{R}^{2n})$ (the L_2-symbols) to the Hilbert space of Hilbert-Schmidt operators acting on $L_2(\mathbb{R}^n)$, and since the product of two Hilbert-Schmidt operators is again a Hilbert-Schmidt operator, we get the estimate (see [7, Lemma 2.12]):

$$\|f \star_\theta g\|_2 \leqslant (2\pi\theta)^{-n/2} \|f\|_2 \|g\|_2.$$

Thus, letting $L_\theta(f) : L_2(\mathbb{R}^{2n}) \ni \psi \mapsto f \star_\theta \psi \in L_2(\mathbb{R}^{2n})$, we see that $L_\theta(f)$ is a bounded operator whenever $f \in L_2(\mathbb{R}^{2n})$, with $\|L_\theta(f)\|_\infty \leqslant (2\pi\theta)^{-n/2}\|f\|_2$. Since the adjoint of $L_\theta(f)$ is $L_\theta(\bar{f})$, we see that

$$\mathscr{A}_0 := \left\{ L_\theta(f),\, \bar{f} = f \in L_2(\mathbb{R}^{2n}) \right\}$$

endowed with the L_2-topology is a real Banach space of bounded operators on $L_2(\mathbb{R}^{2n})$.

Setting $\mathscr{A} = \Delta + \mathscr{A}_0$, with Δ the positive Laplacian on $\mathbb{R}^{2n}$, we have another example of Hilbert-Schmidt compatible operators. It was proved in [7, Lemma 4.3] that

$$\|L_\theta(f)g(-\mathrm{i}\nabla)\|_2 = (2\pi)^{-n}\|g\|_2\|f\|_2.$$

Similarly to Theorem 5.3, we obtain:

THEOREM 5.4. *For any* $\varepsilon > 0$, $\left(L_{g_2^{-1}}, \Delta^{\frac{n}{2}+\varepsilon} + \left\{L_\theta(f), f \in L_2(\mathbb{R}^{2n})_{s.a.}\right\}\right)$ *is HS-compatible.*

5.3. Perturbation via the crossed product.

Let $\mathscr{M}$ be a semi-finite von Neumann algebra acting on a Hilbert space $\mathscr{H}$ and let $\alpha = \{\alpha_t\}_{t\in\mathbb{R}}$ be a weak*-continuous group of $*$-automorphisms on $\mathscr{M}$. For every $a \in \mathscr{M}$, we define a "diagonal" operator $\pi(a)$ in the von Neumann algebra tensor product $\mathscr{B}(L_2(\mathbb{R})) \otimes \mathscr{M}$ by

$$(\pi(a)\rho)(t) := \alpha_{-t}(a)(\rho(t)), \quad \text{for } t \in \mathbb{R},\ \{\rho(t)\}_{t\in\mathbb{R}} \in L_2(\mathbb{R}) \otimes \mathscr{H}.$$

We also define unitary operators λ_t, $t \in \mathbb{R}$,

$$(\lambda_t f)(s) := f(s-t), \quad \text{for } s \in \mathbb{R},\ f \in L_2(\mathbb{R}),$$

and

$$\Lambda_t := \lambda_t \otimes 1 \in \mathscr{B}(L_2(\mathbb{R})) \otimes \mathscr{M}.$$

The operators $\{\pi(x)\}_{x\in\mathscr{M}}$ and $\{\Lambda_t\}_{t\in\mathbb{R}}$ generate the continuous crossed product $\mathscr{R} := \mathscr{M} \rtimes_\alpha \mathbb{R}$. The algebra $\mathscr{R}$ is also generated by the weak-operator integrals

$$\tilde{\pi}(x) := \text{wo-}\int_{\mathbb{R}} \Lambda_t\, \pi(x_t)\, dt,$$

where x is in $K(\mathscr{M})$, the set of weakly-operator continuous functions $\mathbb{R} \ni t \mapsto x_t \in \mathscr{M}$ with compact support [26, Ch. X, Lemma 1.8]. If τ is a normal faithful semi-finite trace on $\mathscr{M}$, then $\hat{\tau}$ given by

$$\hat{\tau}(\tilde{\pi}(x)^*\tilde{\pi}(x)) := \int_{\mathbb{R}} \tau(x_t^* x_t)\, dt, \quad x \in K(\mathscr{M}), \tag{5.3}$$

defines a normal faithful semi-finite trace on $\mathscr{R}$ [27, §2, Lemma 1].

The unitary group $\{\Lambda_t\}_{t\in\mathbb{R}}$ is generated by an unbounded self-adjoint operator

$$D := \frac{1}{2\pi\mathrm{i}}\frac{d}{ds} \otimes 1$$

affiliated with $\mathscr{R}$. Note that for $f \in C_c^2(\mathbb{R})$,

$$f(D) = (2\pi)^{-1/2} \int_{\mathbb{R}} \hat{f}(t)\, e^{\mathrm{i}tD}\, dt = (2\pi)^{-1/2} \int_{\mathbb{R}} \hat{f}(t)\, \Lambda_t\, dt = (2\pi)^{-1/2}\, \tilde{\pi}(\hat{f}1).$$

LEMMA 5.5. *If* $\hat{f} \in L_1(\mathbb{R}) \cap L_2(\mathbb{R})$ *and* $a \in L_2(\mathscr{M})$, *then* $\pi(a)f(D) \in L_2(\mathscr{R})$ *and*

$$\|\pi(a)f(D)\|_2 = (2\pi)^{-1/2}\, \|a\|_2\, \|f\|_2\,.$$

Proof. Let x denote the function $t \mapsto x_t = (2\pi)^{-1/2} a\hat{f}(t)$. Firstly, we verify that $\pi(a)f(D) = \tilde{\pi}(x)$ by comparing the actions of the two elements on every $\rho \in L_2(\mathbb{R}) \otimes \mathscr{H}$. On one hand, for $s \in \mathbb{R}$,

$$\begin{aligned}(2\pi)^{1/2}\,(\pi(a)f(D)\rho)\,(s) &= (2\pi)^{1/2}\alpha_{-s}(a)\,(f(D)\rho)\,(s)\\ &= \alpha_{-s}(a) \int_{\mathbb{R}} \hat{f}(t)\Lambda_t\rho(s)\,dt = \alpha_{-s}(a) \int_{\mathbb{R}} \hat{f}(t)\rho(s-t)\,dt.\end{aligned}$$

On the other hand,

$$(\tilde{\pi}(x)\rho)\,(s) = \int (\pi(x_t)\Lambda_t\rho)\,(s)\,dt = \int_{\mathbb{R}} \alpha_{-s}(x_t)\,(\Lambda_t\rho)\,(s)\,dt = \int_{\mathbb{R}} \alpha_{-s}\,(x_t)\,\rho(s-t)\,dt,$$

which equals $(\pi(a)f(D)\rho)\,(s)$. Thus, to see that $\pi(a)f(D) \in L_2(\mathscr{R})$, we need to show that the trace

$$\hat{\tau}\,(f(D)^*\pi(a^*)\pi(a)f(D)) = \hat{\tau}\,(\tilde{\pi}(x)^*\tilde{\pi}(x))$$

is finite. By (5.3) and by the Plancherel theorem $\int_{\mathbb{R}} |\hat{f}(t)|^2\,dt = \int_{\mathbb{R}} |f(t)|^2\,dt$,

$$\hat{\tau}\,(\tilde{\pi}(x)^*\tilde{\pi}(x)) = \int_{\mathbb{R}} \tau\,(x_t^* x_t)\,dt = \frac{1}{2\pi} \int_{\mathbb{R}} \tau\,(a^*a)\,\overline{\hat{f}(t)}\hat{f}(t)\,dt = \frac{1}{2\pi}\,\|a\|_2^2 \int_{\mathbb{R}} |f(t)|^2\,dt,$$

which is finite since $a \in L_2(\mathscr{M})$ and $f \in L_2(\mathbb{R})$. □

For the positive Laplacian

$$\Delta := -\frac{d^2}{ds^2} \otimes 1,$$

we have the following result:

THEOREM 5.6. *For any* $\varepsilon > 0$, $\left(L_{g_2^{-1}}, \Delta^{\frac{1}{4}+\varepsilon} + \pi(\mathscr{M})\right)$ *is* τ*-HS-compatible.*

Proof. The result follows from Lemma 5.5 and Theorems 3.5 and 3.4. (For more details, see the proof of Theorem 5.3.) □

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