# Spectral shift for relative Schatten class perturbations

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Abstract. We affirmatively settle the question on existence of a real-valued higher order spectral shift function for a pair of self-adjoint operators  $H$  and  $V$  such that  $V$  is bounded and  $V (H - iI)^{-1}$  belongs to a Schatten–von Neumann ideal  $S<sup>n</sup>$  of compact operators in a separable Hilbert space. We also show that the function satisfies the same trace formula as in the known case of  $V \in \mathcal{S}^n$  and that it is unique up to a polynomial summand of order  $n - 1$ . Our result significantly advances earlier partial results where counterparts of the spectral shift function for noncompact perturbations lacked real-valuedness and aforementioned uniqueness as well as appeared in more complicated trace formulas for much more restrictive sets of functions. Our result applies to models arising in noncommutative geometry and mathematical physics.

# 1. Introduction

The spectral shift function originates from the foundational work of M. G. Krein [\[8\]](#page-34-0) which followed I. M. Lifshits' physics research summarised in [\[10\]](#page-34-1). It is a central object in perturbation theory that allows to approximate a perturbed operator function by the unperturbed one while controlling noncommutativity in the remainder. In 1984, Koplienko [\[7\]](#page-34-2) suggested an interesting and useful generalization by considering higher order Taylor remainders and conjecturing existence of higher order spectral shift functions. Many partial results were obtained in that direction, but they were confined to either lower order approximations, weakened trace functionals and representations, or compact perturbations. This paper closes a gap between theory and applications, where perturbations are often noncompact, by proving existence of a higher order spectral shift function under a general condition on a weighted resolvent of the initial operator and obtaining bounds and properties stricter than previously known.

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Our prime result is that, given a self-adjoint operator  $H$  densely defined in a separable Hilbert space  $\mathcal H$  and a bounded self-adjoint operator V on  $\mathcal H$  satisfying

<span id="page-1-3"></span><span id="page-1-0"></span>
$$
V(H - iI)^{-1} \in \mathcal{S}^n,\tag{1}
$$

there exists a real-valued spectral shift function  $\eta_n = \eta_{n,H,V}$  of order n. Namely, the trace formula

$$
\text{Tr}\Big(f(H+V) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} f(H+tV)\Big|_{t=0}\Big) = \int_{\mathbb{R}} f^{(n)}(x) \eta_n(x) \, dx \tag{2}
$$

holds for a wide class of functions f and the function  $\eta_n$  satisfies suitable uniqueness and summability properties and bounds detailed below. The *relative Schatten class condition* [\(1\)](#page-1-0) applies, in particular, to

- <span id="page-1-2"></span><span id="page-1-1"></span>I.  $V \in \mathcal{S}^n$ ;
- <span id="page-1-4"></span>II.  $(H - iI)^{-1} \in \mathcal{S}^n$ ;
- III. inner fluctuations of  $H = D$  in a regular locally compact spectral triple  $(A, \mathcal{H}, D)$  (see Section [5.1\)](#page-30-0);
- IV. differential operators on manifolds perturbed by multiplication operators (see Section [5.2\)](#page-32-0).

To prove our main result, we develop new techniques, which were also applied in the subsequent work  $[12]$  in the setting  $(II)$  to resolve analytical issues occurring in the study of the spectral action in noncommutative geometry. The latter application suggests that our techniques can be used to substantially generalize  $[12,13]$  $[12,13]$  as well as can be useful in other problems of noncommutative geometry.

New and prior results. Under the assumption [\(I\)](#page-1-2), the problem on existence of higher order spectral shift functions was resolved in [\[14\]](#page-34-5). More precisely, [\(2\)](#page-1-3) was established in [\[7,](#page-34-2) [8,](#page-34-0) [14\]](#page-34-5) for  $n = 1$ ,  $n = 2$ ,  $n \ge 3$ , respectively, for important test functions f (see, e.g., [\[21,](#page-35-0) Section 5.5] for details), where the function  $\eta_n = \eta_{n,H,V}$  is unique, realvalued, and satisfies the bound

$$
\|\eta_n\|_1 \leq c_n \|V\|_n^n.
$$

Taylor approximations and respective trace formulas were also derived in the study of the spectral action functional  $\text{Tr}(f(H))$  occurring in noncommutative geo-metry [\[2\]](#page-34-6) for operators H with compact resolvent  $(H - iI)^{-1}$ . The case of [\(II\)](#page-1-1) and functions f in the form  $f(x) = g(x^2)$ , where g is the Laplace transform of a regular Borel measure, was handled in [\[22\]](#page-35-1). The case of compact  $(H - iI)^{-1}$  and  $f \in C_c^{n+1}(\mathbb{R})$  was handled in [\[17,](#page-34-7) [19\]](#page-35-2). In particular, the existence of a locally integrable spectral shift function was established in [\[19\]](#page-35-2).

In our main result, Theorem [4.1,](#page-15-0) given  $n \in \mathbb{N}$  and H, V satisfying [\(1\)](#page-1-0), we establish the existence of a real-valued function  $\eta_n = \eta_{n,H,V}$  such that  $\eta_n \in L^1(\mathbb{R}, \frac{dx}{(1+|x|)^{n+\epsilon}})$ for every  $\varepsilon > 0$  and such that [\(2\)](#page-1-3) holds for every  $f \in \mathfrak{W}_n$ , where the class  $\mathfrak{W}_n$  is given by Definition [3.1.](#page-7-0) In particular,  $\mathfrak{W}_n$  includes all  $(n + 1)$ -times continuously differentiable functions whose derivatives decay at infinity at the rate  $f^{(k)}(x) = O(|x|^{-k-\alpha})$ ,  $k = 0, \ldots, n + 1$ , for some  $\alpha > \frac{1}{2}$  (see Proposition [3.3](#page-7-1) [\(i\)](#page-7-2)). The weighted  $L^1$ -norm of the spectral shift function  $\eta_n$  admits the bound

$$
\int_{\mathbb{R}} |\eta_n(x)| \frac{dx}{(1+|x|)^{n+\varepsilon}} \le c_n (1+\varepsilon^{-1})(1+\|V\|) \|V(H-iI)^{-1}\|_n^n
$$

for every  $\varepsilon > 0$ . Moreover, the locally integrable spectral shift function  $\eta_n$  is unique up to a polynomial summand of degree at most  $n - 1$ .

Below we briefly summarize advantages of our main result in comparison to most relevant prior results. Other results on approximation of operator functions and omitted details can be found in [\[21,](#page-35-0) Chapter 5] and references cited therein.

The existence of a real-valued function  $\eta_1 \in L^1(\mathbb{R}, \frac{dx}{1+x^2})$  satisfying the trace formula [\(2\)](#page-1-3) with  $n = 1$  for bounded rational functions was established in [\[9,](#page-34-8) Theorem 3] (see also [\[26,](#page-35-3) p. 48, Corollary 0.9.5]). The formula [\(2\)](#page-1-3) was extended to twice-differentiable f with bounded  $f'$ ,  $f''$  such that

<span id="page-2-0"></span>
$$
\frac{d^k}{dx^k}(f(x) - c_f x^{-1}) = O(|x|^{-k-1-\varepsilon}) \quad \text{as } |x| \to \infty, \, k = 0, 1, 2, \, \varepsilon > 0,\qquad(3)
$$

where  $c_f$  is a constant, in [\[26,](#page-35-3) p. 47, Theorem 0.9.4]. It was shown in [\[24,](#page-35-4) Section 8.8(3)] that  $\eta_1 \in L^1(\mathbb{R}, \frac{dx}{(1+|x|)})$  $\frac{dx}{(1+|x|)^{1+\epsilon}}$  for  $\varepsilon > 0$ . The respective function  $\eta_1$  was determined by [\(2\)](#page-1-3) uniquely up to a constant summand. We prove that [\(2\)](#page-1-3) with  $n = 1$ holds for all  $\mathfrak{W}_1$ , which contains all functions satisfying [\(3\)](#page-2-0) (see Proposition [3.3](#page-7-1)[\(i\)](#page-7-2)) as well as functions not included in [\(3\)](#page-2-0) (see, e.g., Remark [3.4\)](#page-8-0).

In [\[11,](#page-34-9) Corollary 3.7], the trace formula [\(2\)](#page-1-3) with  $n = 2$  and real-valued  $\eta_2 \in$  $L^1(\mathbb{R}, \frac{dx}{(1+x^2)^2})$  was proved for a set of functions including Schwartz functions along with span $\{(z-\cdot)^{-k} : \text{Im}(z) \neq 0, k \in \mathbb{N}, k \geq 2\}$ . The respective  $\eta_2 \in L^1(\mathbb{R}, \frac{dx}{(1+x^2)^2})$ was determined by [\(2\)](#page-1-3) uniquely up to a linear summand. We prove that  $(2)$  with  $n = 2$  holds for all  $f \in \mathfrak{W}_2$ , which contains the functions  $(z - \cdot)^{-1}$ , Im $(z) \neq 0$  not included in [\[11,](#page-34-9) Corollary 3.7] and the Schwartz functions included in [\[11,](#page-34-9) Corollary 3.7], and that  $\eta_2$  is integrable with a significantly smaller weight, namely,  $\eta_2 \in$  $L^1(\mathbb{R}, \frac{dx}{(1+|x|)}$  $\frac{dx}{(1+|x|)^{2+\varepsilon}}$ ) for  $\varepsilon > 0$ .

Let  $n \ge 2$ . The existence of a complex-valued  $\tilde{\eta}_n \in L^1(\mathbb{R}, \frac{dx}{(1+x^2)^{n/2}})$  satisfying the trace formula

$$
\operatorname{Tr}\left(f(H+V) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} f(H+tV)\Big|_{t=0}\right)
$$
  
= 
$$
\int_{\mathbb{R}} \frac{d^{n-1}}{dx^{n-1}} ((x-i)^{2n} f'(x)) \tilde{\eta}_n(x) dx
$$
 (4)

for a set of functions f including span $\{(z-\cdot)^{-k}, \text{Im}(z) > 0, k \in \mathbb{N}, k \ge 2n\}$  was established in [\[4,](#page-34-10) Theorem 4.6] (see also [4, Remark 4.8 (ii)]). The weighted  $L^1$ -norm of  $\tilde{\eta}_n$  satisfies the bound

$$
\int_{\mathbb{R}} |\tilde{\eta}_n(x)| \frac{dx}{(1+x^2)^{\frac{n}{2}}} \le c_n (1+||V||)^{n-1} ||V(H-iI)^{-1}||_n^n.
$$

As distinct from the aforementioned result of [\[4\]](#page-34-10) for  $n \ge 2$ , the function  $\eta_n$  in our main result is real-valued and satisfies the simpler trace formula [\(2\)](#page-1-3) for the larger class  $\mathfrak{W}_n$  of functions f described in terms of familiar function classes. Moreover, the set of functions  $\mathfrak{W}_n$  is large enough to ensure the uniqueness of  $\eta_n$  up to a polynomial term of degree at most  $n - 1$ .

Other assumptions on  $H$  and  $V$ , each having its merits and limitations, were also considered in the literature. For instance, the existence of a nonnegative function  $\eta_2 =$  $\eta_{2,H,V} \in L^1(\mathbb{R}, \frac{dx}{(1+x^2)^{\gamma}}), \gamma > 1/2$ , satisfying the trace formula [\(2\)](#page-1-3) with  $n = 2$  for bounded rational functions  $f$  was established in [\[7,](#page-34-2) Theorem 2] under the assumption  $V|H - iI|^{-\frac{1}{2}} \in \mathcal{S}^2$ . A more relaxed condition  $(H + V - iI)^{-1} - (H - iI)^{-1} \in$  $S<sup>n</sup>$  was traded off for a more restrictive set of functions f and, when  $n \ge 2$ , for more complicated trace formulas where both the left and right-hand sides of [\(2\)](#page-1-3) are modified. The respective results for  $n = 1$  can be found in [\[9,](#page-34-8) Theorem 3] and [\[25,](#page-35-5) Theorem 2.2]; for  $n = 2$  in [\[11,](#page-34-9) Theorem 3.5 and Corollary 3.6]; for  $n \ge 2$  in [\[15,](#page-34-11) Theorem 3.5] and [\[18\]](#page-34-12).

Methods. The major technical tools and novelty of our approach are briefly discussed below.

The technical scheme leading to the representation  $(2)$  under the assumption  $(1)$ is more subtle than the one under the assumption [\(I\)](#page-1-2). The derivatives and Taylor approximations of operator functions are known to be expressible in terms of multiple operator integrals (see Theorems [3.12](#page-14-0) and [3.13\)](#page-15-1). The prime technique to handle these multiple operator integrals (see Theorem [3.7\)](#page-10-0) only applies to compact perturbations satisfying  $(I)$ . To bridge the gap between existing results for  $(I)$  and our setting  $(I)$  we impose suitable weights on the perturbations and involve multi-stage approximation arguments for functions and perturbations.

In Theorem [3.10](#page-12-0) we create Schatten class perturbations out of relative Schatten class perturbations [\(1\)](#page-1-0) inside a multiple operator integral whose integrand is the *n*-th order divided difference  $f^{[n]}$  of a function  $f \in C^n(\mathbb{R})$  satisfying the properties  $f^{(k)}(x) = o(|x|^{-k})$ difference  $f^{[n]}$  of a function  $f \in C^n(\mathbb{R})$  satisfyi<br>  $|x| \to \infty$ ,  $k = 0, ..., n$ , and  $\widehat{f^{(n)}} \in L^1(\mathbb{R})$ .

Our Theorem [3.10](#page-12-0) significantly generalizes and extends earlier attempts in that direction made in [\[17,](#page-34-7) Lemma 3.6], [\[19,](#page-35-2) Proposition 2.7], and [\[4,](#page-34-10) Lemma 4.1].

The proof of Theorem [3.10](#page-12-0) involves the introduction of novel function classes (see Definition [3.1,](#page-7-0) [\(9\)](#page-8-1), and [\(10\)](#page-8-2)), approximation arguments (see Lemma [3.5\)](#page-8-3), and analysis of multilinear operator integrals.

Based on the aforementioned results and analysis of distributions, in Proposition [4.2](#page-16-0) we establish the trace formula

<span id="page-4-0"></span>
$$
\text{Tr}\Big(f(H+V) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} f(H+tV)\Big|_{t=0}\Big) = \int_{\mathbb{R}} f^{(n)}(x) \, d\mu_n(x) \qquad (5)
$$

for every  $f \in \mathfrak{W}_n$ , where  $\mu_n$  is a Borel measure determined uniquely up to an absolutely continuous term whose density is a polynomial of degree at most  $n - 1$  and such that for every  $\varepsilon > 0$  the measure  $(x - i)^{-n - \varepsilon} d\mu_n(x)$  is finite and satisfies

$$
\|(-i)^{-n-\varepsilon} d\mu_n\| \le c_n (1+\varepsilon^{-1})(1+\|V\|) \|V(H-iI)^{-1}\|_n^n. \tag{6}
$$

In order to obtain absolute continuity of  $\mu_n$  (and hence obtain a spectral shift *function*), we apply the change of variables provided by Theorem [3.10](#page-12-0) again, this time to multiple operator integrals of order  $n - 1$ . This entails new terms for which the trace is defined only when perturbations satisfy additional summability requirements. We establish an auxiliary result for finite rank perturbations in Proposition [4.2](#page-21-0) and then extend it to relative Schatten class perturbations appearing in our main result with help of two new approximation results, one for operators obtained in Lemma [4.8](#page-23-0) and the other for Taylor remainders obtained in Lemma [4.9.](#page-24-0) In order to apply those approximation results, in Lemma [4.5](#page-21-1) we derive a new representation for the remainder of the Taylor approximation of  $f(H + V)$  in terms of handy components that are continuous in  $V$  in a very strong sense.

In order to strengthen [\(5\)](#page-4-0), in Proposition [4.4](#page-21-2) we establish another weaker version of [\(2\)](#page-1-3) for  $f \in C_c^{n+1}(\mathbb{R})$ , where on the left-hand side we have a certain component of the Taylor remainder and on the right-hand side in place of  $f$  we have its product with some complex weight. By combining advantages of the results of Propositions [4.2](#page-16-0) and [4.4](#page-21-2) we derive the trace formula [\(2\)](#page-1-3).

Examples. The relative Schatten class condition [\(1\)](#page-1-0) arises in noncommutative geometry; see, for instance,  $[22, 23]$  $[22, 23]$ . In that setting, H is a generalized Dirac operator occurring in a (possibly non-unital) spectral triple and  $V$  a generalized vector potential [\[5,](#page-34-13) Section IV.1], which is also known as an inner fluctuation or Connes' differential one-form  $[2,22]$  $[2,22]$ . For unital spectral triples, the condition  $(II)$ , which is known as finite summability, is often assumed. For non-unital spectral triples, conditions similar to [\(III\)](#page-1-4) are discussed in Section [5.1.](#page-30-0) Both in the unital and non-unital case, it is important to relax assumptions on the function  $f$  appearing in the spectral action [\[2\]](#page-34-6) since that function might be prescribed by the model [\[3\]](#page-34-14). Sometimes, it is impossible or at least inconvenient to assume that  $f$  is given by a Laplace transform, as it was done in [\[22\]](#page-35-1), and a general class of functions considered in this paper is more beneficial.

The condition [\(1\)](#page-1-0) is also satisfied by many Dirac as well as random and deterministic Schrödinger operators H with  $L^p$ -potentials V. Appearance of such operators in problems of mathematical physics is discussed in, for instance, [\[20,](#page-35-7)[26\]](#page-35-3) and references cited therein. Sufficient conditions for [\(1\)](#page-1-0) are discussed in Section [5.](#page-30-1)

# 2. Notations

Let  $\mathcal H$  be a separable Hilbert space,  $\mathcal B(\mathcal H)$  the  $C^*$ -algebra of all bounded linear operators on H, and  $\mathcal{B}(\mathcal{H})_{sa}$  the subset of all self-adjoint operators in  $\mathcal{B}(\mathcal{H})$ . For  $p \in$  $[1, \infty)$ , we denote the respective Schatten–von Neumann ideal of compact operators on  $\mathcal H$  by  $S^p$  and briefly call it the Schatten p-class. Basic properties of Schatten– von Neumann ideals can be found in, for instance, [\[16,](#page-34-15) [21\]](#page-35-0). In some cases it will also be convenient to denote  $S^{\infty} := \mathcal{B}(\mathcal{H})$ .

Let N denote the positive natural numbers and let  $n \in \mathbb{N}$ . When H is a selfadjoint operator densely defined in  $H$ , we briefly write  $H$  *is a self-adjoint operator in*  $H$ . Given a self-adjoint operator H in  $H$  and  $V \in \mathcal{B}(H)$ , we denote

$$
\widetilde{V} := V(H - iI)^{-1}.
$$

Throughout the paper we will also use the notations

$$
u(\lambda) := \lambda - i
$$

and  $u^{-k}(x) := (u(x))^{-k}$ . If  $H_0, \ldots, H_m$  are self-adjoint operators in  $\mathcal{H}$ , and  $V_1, \ldots,$  $V_m$  are bounded operators, we denote

$$
\widetilde{V}_j := V_j u^{-1}(H_j) = V_j (H_j - iI)^{-1}.
$$

Given two Banach spaces  $X$  and  $Y$ , let  $\mathcal{B}(\mathcal{X}, \mathcal{Y})$  denote the Banach space of all bounded linear operators mapping X to Y. For  $T \in \mathcal{B}(\mathcal{X}, \mathcal{Y})$ ; we denote its norm by  $||T||_{\mathcal{X}\rightarrow\mathcal{Y}}.$ 

We denote positive constants by letters  $c, C$  with subscript indicating dependence on their parameters. For instance, the symbol  $c_{\alpha}$  denotes a constant depending only on the parameter  $\alpha$ .

**Function spaces.** Let  $C_0 = C_0(\mathbb{R})$  denote the space of continuous functions on  $\mathbb{R}$ decaying to 0 at infinity,  $C_c = C_c(\mathbb{R})$  the space of compactly supported continuous functions on  $\mathbb{R}$ ,  $C_c^n$  the class of *n* times continuously differentiable functions in  $C_c$ , and  $C_c^n[-a, a]$  the class of functions in  $C_c^n$  whose support is contained in  $[-a, a]$ . Let  $C_b^n$  denote the subset of  $C^n$  of such f for which  $f^{(n)}$  is bounded and let  $C_0^n$  denote the subset of  $C^n$  of such f for which  $f^{(n)} \in C_0(\mathbb{R})$ . We write  $f(x) = O(g(x))$  if there exists  $M > 0$  such that  $|f(x)| \leq Mg(x)$  for all x outside a compact set. We write  $f(x) = o(g(x))$  if, for all  $\varepsilon > 0$ , we have  $|f(x)| \leq \varepsilon g(x)$  for all x outside a compact set depending on  $\varepsilon$ .

Let  $L^p$  denote the space of measurable f for which  $|f|^p$  is Lebesgue integrable on  $\mathbb R$  equipped with the standard norm  $|| f ||_p = || f ||_{L^p} := (\int_{\mathbb R} |f(x)|^p dx)^{1/p}$ ,  $1 \leq p < \infty$ , and let  $L^{\infty}$  denote the space of essentially bounded functions on R equipped with the ess sup norm  $\|\cdot\|_{\infty}$ . Let  $L^1_{\text{loc}}$  denote the space of functions locally integrable on R equipped with the seminorms  $f \mapsto \int_{-a}^{a} |f(x)| dx$ ,  $a > 0$ . By  $\ell^p(L^2(\mathbb{R}^d))$ , where  $p \geq 1$ , we denote the space of functions consisting of those measurable functions  $f: \mathbb{R}^d \to \mathbb{C}$  for which

$$
\|f\|_{\ell^p(L^2(\mathbb{R}^d))}^p := \sum_{k \in \mathbb{Z}^d} \left( \int\limits_{(0,1)^d + k} |f(x)|^2 \, dx \right)^{\frac{p}{2}} < \infty. \tag{7}
$$

Whenever we write  $\hat{f} \in L^1$ , it is implicitly assumed that  $f \in C_0 \subseteq S'$ , in order to define the Fourier transform. This can be done without loss of generality by the Riemann–Lebesgue lemma.

We recall that the divided difference of the zeroth order  $f^{[0]}$  is the function f itself. Let  $\lambda_0, \lambda_1, \ldots, \lambda_n$  be points in  $\mathbb R$  and let  $f \in C^n(\mathbb R)$ . The divided difference  $f^{[n]}$  of order *n* is defined recursively by

$$
f^{[n]}(\lambda_0,\ldots,\lambda_n)=\lim_{\lambda\to\lambda_n}\frac{f^{[n-1]}(\lambda_0,\ldots,\lambda_{n-2},\lambda)-f^{[n-1]}(\lambda_0,\ldots,\lambda_{n-2},\lambda_{n-1})}{\lambda-\lambda_{n-1}}.
$$

# 3. Auxiliary technical results

In this section we set a technical foundation for the proof of our main result.

### 3.1. New function classes

In this section we introduce a new class of functions  $\mathfrak{W}_n$ , for which our main result holds, along with auxiliary classes  $\mathfrak{B}_n$  and  $\mathfrak{b}_n$  and derive their properties.

<span id="page-7-0"></span>**Definition 3.1.** Let  $\mathfrak{W}_n$  denote the set of functions  $f \in C^n(\mathbb{R})$  such that<br>i.  $\widehat{f^{(k)}u^k} \in L^1(\mathbb{R}), k = 0, \ldots, n$ ,

i. 
$$
\bar{f}^{(k)}u^{\bar{k}} \in L^1(\mathbb{R}), k = 0, ..., n,
$$
  
ii.  $f^{(k)} \in L^1(\mathbb{R}, (1+|x|)^{k-1} dx), k = 1, ..., n.$ 

The following sufficient condition for integrability of the Fourier transform of a function is a standard exercise and, thus, its proof is omitted.

<span id="page-7-3"></span>**Lemma 3.2.** *If*  $f \in L^2(\mathbb{R}) \cap C^1(\mathbb{R})$  *and*  $f' \in L^2(\mathbb{R})$ *, then*  $\hat{f} \in L^1(\mathbb{R})$ *.* 

<span id="page-7-2"></span><span id="page-7-1"></span>**Proposition 3.3.** *Let*  $n \in \mathbb{N}$ *. Then, the following assertions hold.* 

- i. For every  $\alpha > \frac{1}{2}$ ,  $\mathfrak{W}_n \supseteq \{f \in C^{n+1}: f^{(k)}(x) = O(|x|^{-k-\alpha}) \text{ as } |x| \to \infty, \}$  $k = 0, \ldots, n + 1$ .
- <span id="page-7-5"></span>ii. *Furthermore,*

$$
\mathfrak{W}_n \subseteq \{f \in C^n : f^{(k)}, \widehat{f^{(k)}} \in L^1(\mathbb{R}), k = 1, \ldots, n\}.
$$

*Proof.* The inclusion in (i) is straightforward, as it follows from Lemma [3.2.](#page-7-3)

(ii) The properties  $f^{(k)}$ is straight<br> $\widehat{f^{(n)}} \in L$ <sup>1</sup>( $\mathbb{R}$ ),  $k = 1, \ldots, n$  follow immediately from the (ii) The properties  $f^{(k)}$ ,  $f^{(n)} \in L$ <br>definition of  $\mathfrak{W}_n$ . To prove  $\widehat{f^{(k)}} \in L$  $\mathbf{1}(\mathbb{R}), k = 1, \ldots, n - 1$ , firstly we confirm that

$$
f^{(k)}u^k \in C_0, \quad k = 1, \dots, n-1,\tag{8}
$$

for every  $f \in \mathfrak{W}_n$ .

Fix  $k \in \{2, \ldots, n\}$  and let

<span id="page-7-4"></span>
$$
g = f^{(k-1)}u^{k-1}.
$$

Then, by the definition of the class  $\mathfrak{W}_n$ ,

$$
g' = f^{(k)}u^{k-1} + (k-1)f^{(k-1)}u^{k-2} \in L^1(\mathbb{R}).
$$

It follows that both  $\lim_{x\to\infty} g(x)$  and  $\lim_{x\to\infty} g(x)$  exist. Suppose that

$$
\lim_{x \to \infty} g(x) \neq 0.
$$

Then there exist  $L, c > 0$  such that for all  $x \geq L$  we have  $|g(x)| \geq c$ . Therefore,

$$
c\int_{L}^{\infty} |u^{-1}(x)| dx \leq \int_{L}^{\infty} |f^{(k-1)}(x)u^{k-2}(x)| dx < \infty,
$$

which is impossible. Hence,  $\lim_{x\to\infty} g(x) = 0$  and, similarly,  $\lim_{x\to\infty} g(x) = 0$ . Thus,  $(8)$  holds.

From [\(8\)](#page-7-4), we deduce that  $f^{(k)} \in L^{\infty}(\mathbb{R})$ ,  $k = 1, ..., n - 1$ . By the definition of  $\mathfrak{W}_n$ , we also have  $f^{(n)} \in L^{\infty}(\mathbb{R})$ . Combining the latter with  $f^{(k)} \in L^1(\mathbb{R})$ ,  $k =$  $1, \ldots, n$ , implies  $f^{(k)} \in L^2$  $\exists L^{\infty}(\mathbb{R})$ . Combining the latter with  $f^{(k)} \in L^1(\mathbb{R})$ ,<br> $(\mathbb{R}), k = 1, ..., n$ . Hence, by Lemma [3.2,](#page-7-3)  $\widehat{f^{(k)}} \in L$  $^{1}(\mathbb{R})$ for  $k = 1, ..., n - 1$ . Therefore, the proof of (ii) is complete.

<span id="page-8-0"></span>**Remark 3.4.** It follows from Proposition [3.3](#page-7-1) [\(i\)](#page-7-2) that  $\mathfrak{W}_n$  contains all bounded rational functions except for linear combinations with constant functions, which are trivial in the context of our paper. In particular,  $\mathfrak{W}_n$  contains the space span $\{(z - \cdot)^{-k},\}$  $\text{Im}(z) > 0, k \in \mathbb{N}, k \ge 2n$  considered in [\[4\]](#page-34-10). In addition,  $\mathfrak{W}_n$  contains all Schwartz functions and every  $f \in C^{n+1}$  such that  $f(x) = |x|^{-\alpha}$  outside a bounded neighborhood of zero for some  $\alpha > \frac{1}{2}$ .

We will need the auxiliary function classes

$$
\mathfrak{B}_n := \{ f \in C^n : f^{(k)} u^k \in C_0(\mathbb{R}), \ k = 0, \dots, n, \ \widehat{f^{(n)}} \in L^1(\mathbb{R}) \} \tag{9}
$$

and

$$
\mathfrak{b}_n := \{ f \in \mathfrak{B}_n : \widehat{f^{(p)}u^p} \in L^1(\mathbb{R}), \ p = 0, \dots, n \}. \tag{10}
$$

It follows from Definition [3.1,](#page-7-0) Proposition  $3.3$  [\(ii\)](#page-7-5), and [\(8\)](#page-7-4) that

<span id="page-8-2"></span><span id="page-8-1"></span>
$$
\mathfrak{W}_n\subset \mathfrak{B}_n.
$$

We also have the following result relating  $b_n$  and  $\mathfrak{B}_n$ .

<span id="page-8-3"></span>**Lemma 3.5.** *The space*  $b_n$  *is dense in*  $\mathcal{B}_n$  *with respect to the norm* 

$$
|| f ||_{\mathfrak{B}_n} := \sum_{p=0}^n || f^{(p)} u^p ||_{\infty} + || \widehat{f^{(n)}} ||_1.
$$

*Proof.* Let  $f \in \mathfrak{B}_n$ . Fix a Schwartz function  $\phi$  such that  $\hat{\phi} \in C_c^{\infty}(\mathbb{R})$  and  $\phi(0) = 1$ . For every  $k \in \mathbb{N}$ , define

$$
\phi_k(x) := \phi(x/k), \quad x \in \mathbb{R}.
$$

We note that  $\{\widehat{\phi_k}\}_{k=1}^{\infty}$  is an approximate identity. In particular, it satisfies the property

$$
\|\widehat{\phi_k} * g - g\|_1 \to 0 \quad \text{as } k \to \infty \tag{11}
$$

for every  $g \in L^1$ . Define

<span id="page-9-4"></span>
$$
f_k := \phi_k f.
$$

Because every  $\phi_k^{(m)}$  $\binom{m}{k}$  is of rapid decrease, it is obvious that

$$
f_k^{(p)}u^p = \sum_{m=0}^p {p \choose m} \phi_k^{(m)} f^{(p-m)} u^p
$$

is integrable for every  $p \in \{0, \ldots, n\}$ . By Lemma [3.2](#page-7-3) and the rapid decrease of every  $\phi_k^{(m)}$ rable for every  $p \in \{0, \ldots, n\}$ . By Lemma 3.2 and the rapid decrease of  $\binom{m}{k}$ , we obtain that  $\widehat{f_k^{(p)}u^p} \in L^1$  for every  $p \in \{0, \ldots, n-1\}$ . In the same way, we obtain that  $(f^{(p)}\phi_k^{(n-p)})$  $\binom{n-p}{k}$  $u^n$ )<sup> $\hat{ } \in L^1$ </sup> for every  $p \in \{0, \ldots, n-1\}$ . Moreover, we have  $(f^{(n)}\phi_k u^n)$  $(f^{(p)}\phi_k^{(n-p)}u^n)^{\hat{}} \in L^1$  for ever<br>  $f^{(n)} \ast \widehat{\phi_k u^n} \in L^1$ . Hence,

$$
\widehat{f_k^{(n)}u^n} = \sum_{p=0}^n \binom{n}{p} (f^{(p)}\phi_k^{(n-p)}u^n)^{\hat{}} \in L^1.
$$

We conclude that  $f_k \in \mathfrak{b}_n$ .

In order to prove that  $\| f^{(p)} u^p - f^{(p)}_k\|$  $\int_k^{\cdot}(p)u^p\|_{\infty} \to 0$  as  $k \to \infty$ , we write

$$
\|f^{(p)}u^p - f_k^{(p)}u^p\|_{\infty}
$$
  
\n
$$
\leq \|(1 - \phi_k)f^{(p)}u^p\|_{\infty} + \sum_{m=1}^p {p \choose m} \|\phi_k^{(m)}u^m f^{(p-m)}u^{p-m}\|_{\infty}.
$$
 (12)

Since  $f^{(p)}u^p \in C_0(\mathbb{R})$ , we obtain

<span id="page-9-3"></span><span id="page-9-0"></span>
$$
\|(1 - \phi_k)f^{(p)}u^p\|_{\infty} \to 0 \quad \text{as } k \to \infty.
$$
 (13)

By using  $\phi_k^{(m)}$  $\binom{m}{k}(x) = \phi^{(m)}(x/k)/k^m$ , we obtain

$$
|\phi_k^{(m)}(x)u^m(x)| \le \sqrt{2}^m \|\phi^{(m)}\|_{\infty} k^{-m/2} \quad \text{for } x \in [-\sqrt{k}, \sqrt{k}] \tag{14}
$$

and

<span id="page-9-2"></span><span id="page-9-1"></span>
$$
\|\phi_k^{(m)}u^m\|_{\infty} \le \sqrt{2}^m \|\phi^{(m)}u^m\|_{\infty}.
$$
 (15)

We now analyze the terms on the right-hand side of [\(12\)](#page-9-0) as  $k \to \infty$ . By [\(14\)](#page-9-1), [\(15\)](#page-9-2), and the assumption  $f^{(p-m)}u^{p-m} \in C_0$ , we obtain  $\|\phi_k^{(m)}\|$  $\int_{k}^{(m)} u^{m} f^{(p-m)} u^{p-m} \|_{\infty} \to 0$  as  $k \to \infty$ . Combining the latter with [\(12\)](#page-9-0) and [\(13\)](#page-9-3) implies

$$
\|f^{(p)}u^p - f_k^{(p)}u^p\|_{\infty} \to 0 \quad \text{as } k \to \infty, \quad p = 0, \dots, n.
$$

We are left to prove that  $\|\widehat{f^{(n)}} - \widehat{f_k^{(n)}}\|_1 \to 0$ . Applying

<span id="page-10-1"></span>
$$
f_k^{(n)} = \sum_{m=0}^{n} {n \choose m} \phi_k^{(m)} f^{(n-m)}
$$

along with standard properties of the Fourier transform and convolution yields

$$
\|\widehat{f^{(n)}} - \widehat{f_k^{(n)}}\|_1 \le \|\widehat{f^{(n)}} - \widehat{\phi_k} * \widehat{f^{(n)}}\|_1 + \sum_{m=1}^n {n \choose m} \frac{\|\widehat{\phi^{(m)}}\|_1}{k^m} \|\widehat{f^{(n-m)}}\|_1. \tag{16}
$$

The first term on the right-hand side of [\(16\)](#page-10-1) converges to 0 as  $k \to \infty$  by [\(11\)](#page-9-4) applied to  $g = \widehat{f^{(n)}}$ . The other terms on the right-hand side of [\(16\)](#page-10-1) converge to 0 as  $k \to \infty$ because  $1/k^m \rightarrow 0$ .  $\blacksquare$ 

## 3.2. Multilinear operator integration

In this section we recall known as well as establish new technical results on operator integration that are important in the proof of our main theorem. An interested reader can find a more detailed discussion of the known results in [\[21\]](#page-35-0).

The following multilinear operator integral was introduced in [\[14\]](#page-34-5) (see also [\[21,](#page-35-0) Definition 4.3.3]).

<span id="page-10-2"></span>**Definition 3.6.** For  $n \in \mathbb{N}$ , let  $\phi: \mathbb{R}^{n+1} \to \mathbb{C}$  be a bounded Borel function and fix  $\alpha, \alpha_1, \ldots, \alpha_n \in [1, \infty]$  such that  $\frac{1}{\alpha} = \frac{1}{\alpha_1} + \cdots + \frac{1}{\alpha_n}$ . Let  $H_0, \ldots, H_n$  be self-adjoint operators in  $\mathcal{H}$ . Denote  $E^j_{l,m} := E_{H_j}([\frac{l}{m}, \frac{l+1}{m})]$  $\frac{+1}{m}$ )). If for all  $V_j \in \mathcal{S}^{\alpha_j}$ ,  $j = 1, \ldots, n$ , the iterated limit

$$
T_{\phi}^{H_0,...,H_n}(V_1,...,V_n)
$$
  
 :=  $\lim_{m \to \infty} \lim_{N \to \infty} \sum_{|l_0|,...,|l_n| < N} \phi\left(\frac{l_0}{m}, \dots, \frac{l_n}{m}\right) E_{l_0,m}^0 V_1 E_{l_1,m}^1 \dots V_n E_{l_n,m}^n$ 

exists in  $S^{\alpha}$ , then the transformation  $T_{\phi}^{H_0,...,H_n}$ , which belongs to  $\mathcal{B}(S^{\alpha_1} \times \cdots \times S^{\alpha_n})$ ,  $S^{\alpha}$ ) by the Banach–Steinhaus theorem, is called a *multilinear operator integral*.

We write  $T_{\phi}^{H_0,...,H_n} \in \mathcal{B}(\mathcal{S}^{\alpha_1} \times \cdots \times \mathcal{S}^{\alpha_n}, \mathcal{S}^{\alpha})$  to indicate that  $T_{\phi}^{H_0,...,H_n}$  exists in the sense of Definition [3.6.](#page-10-2) The transformation given by the latter definition satisfies the following powerful estimate.

<span id="page-10-0"></span>**Theorem 3.7.** Let  $\alpha, \alpha_1, \ldots, \alpha_n \in (1, \infty)$  be such that  $\frac{1}{\alpha} = \frac{1}{\alpha_1} + \cdots + \frac{1}{\alpha_n}$ . If  $f \in C^n$ *is such that*  $f^{(n)} \in C_b$ *, then*  $T^{H_0,...,H_n}_{f^{[n]}} \in \mathcal{B}(\mathcal{S}^{\alpha_1} \times \cdots \times \mathcal{S}^{\alpha_n}, \mathcal{S}^{\alpha})$  and

$$
\|T_{f^{[n]}}^{H_0,\dots,H_n}\|_{\mathcal{S}^{\alpha_1}\times\cdots\times\mathcal{S}^{\alpha_n}\to\mathcal{S}^{\alpha}} \leq c_{\alpha_1,\dots,\alpha_n} \|f^{(n)}\|_{\infty}.
$$
 (17)

*Proof.* The result for  $H_0 = \cdots = H_n$  is proved in [\[14,](#page-34-5) Theorem 5.6]. Its extension to the case of distinct  $H_0, \ldots, H_n$  is explained in the proof of [\[21,](#page-35-0) Theorem 4.3.10].

The domain of  $T_{\phi}^{H_0,...,H_n}$  extends to  $\mathcal{B}(\mathcal{H})^{\times n} = \mathcal{S}^{\infty} \times \cdots \times \mathcal{S}^{\infty}$  for functions  $\phi$ admitting a certain separation of variables. The proof of the following result can be found in [\[14,](#page-34-5) Lemma 3.5].

<span id="page-11-1"></span>**Theorem 3.8.** Let  $H_0, \ldots, H_n$  be self-adjoint operators in  $\mathcal{H}$ . Let  $\phi: \mathbb{R}^{n+1} \to \mathbb{C}$  be *a function admitting the representation*

$$
\phi(\lambda_0,\ldots,\lambda_n) = \int\limits_{\Omega} \alpha_0(\lambda_0,s)\ldots\alpha_n(\lambda_n,s) \,d\nu(s),\tag{18}
$$

*where*  $(\Omega, \nu)$  *is a finite measure space,* 

<span id="page-11-0"></span>
$$
\alpha_j(\cdot,s)\colon\mathbb{R}\to\mathbb{C},\quad s\in\Omega,
$$

are bounded continuous functions, and there is a sequence  $\{\Omega_k\}_{k=1}^\infty$  of growing meas*urable subsets of*  $\Omega$  *such that*  $\Omega = \cup_{k=1}^{\infty} \Omega_k$  *and the families* 

$$
\{\alpha_j(\cdot,s)\}_{s\in\Omega_k},\quad j=0,\ldots,n
$$

are uniformly bounded and uniformly equicontinuous. Then,  $T_{\phi}^{H_0,...,H_n} \in \mathcal{B}(\mathcal{S}^{\alpha_1} \times$  $\cdots \times \mathcal{S}^{\alpha_n}, \mathcal{S}^{\alpha}$  for all  $\alpha, \alpha_j \in [1, \infty]$  with  $\frac{1}{\alpha_1} + \cdots + \frac{1}{\alpha_n} = \frac{1}{\alpha}$ , as well as

$$
T_{\phi}^{H_0,\ldots,H_n}(V_1,\ldots,V_n)(y)
$$
  
=  $\int_{\Omega} \alpha_0(H_0,s) V_1 \alpha_1(H_1,s) \ldots V_n \alpha_n(H_n,s) y \, d\nu(s), \quad y \in \mathcal{H},$ 

*and*

$$
||T_{\phi}^{H_0,\ldots,H_n}||_{\mathcal{S}^{\alpha_1}\times\cdots\times\mathcal{S}^{\alpha_n}\to\mathcal{S}^{\alpha}} \leq \inf \int_{\Omega} \prod_{j=0}^n ||\alpha_j(\cdot,s)||_{\infty} d|\nu|(s),
$$

*where the infimum is taken over all possible representations* [\(18\)](#page-11-0)*.*

We will also need the following particular case of Theorem [3.8.](#page-11-1)

<span id="page-11-3"></span>**Theorem 3.9.** *If*  $f \in C^n$  *and*  $\widehat{f^{(n)}} \in L^1$ , *then*  $\phi = f^{[n]}$  *satisfies the assumptions of Theorem* [3.8](#page-11-1) *and, for all*  $\alpha, \alpha_j \in [1, \infty]$  *with*  $\frac{1}{\alpha_1} + \cdots + \frac{1}{\alpha_n} = \frac{1}{\alpha}$ ,

<span id="page-11-2"></span>
$$
||T_{f^{[n]}}^{H_0,...,H_n}||_{\mathcal{S}^{\alpha_1}\times\cdots\times\mathcal{S}^{\alpha_n}\to\mathcal{S}^{\alpha}} \leq \frac{1}{n!}||\widehat{f^{(n)}}||_1.
$$
 (19)

*Proof.* Let  $\phi = f^{[n]}$ , where  $f \in C^n$ and  $\widehat{f^{(n)}} \in L$ <sup>1</sup>. A straightforward induction argument (see, e.g., the proofs of [\[14,](#page-34-5) Lemma 5.1 and Lemma 5.2]) gives

$$
f^{[n]}(\lambda_0,\ldots,\lambda_n) = \int\limits_{\Delta_n} \int\limits_{\mathbb{R}} e^{its_0\lambda_0}\ldots e^{its_n\lambda_n} \widehat{f^{(n)}}(t) dt d\sigma(s),
$$
 (20)

where  $\Delta_n = \{s = (s_0, \ldots, s_n) \in \mathbb{R}^{n+1}_{\geq 0} : \sum_{j=0}^n s_j = 1\}$  is the *n*-simplex,  $d\sigma$  is the Lebesgue measure on  $\Delta_n$ , and dt is the Lebesgue measure on  $\mathbb R$ . That is,  $f^{[n]}$  admits a representation of the form (18), where  $(\Omega, \nu) = (\Delta_n \times \mathbb R, d\sigma \times (\widehat{f^{(n)}}(t) dt))$ . Since Lebesgue measure on  $\Delta_n$ , and dt is the Lebesgue measure on R. That is,  $f^{[n]}$  admits a representation of the form (18), where  $(\Omega, \nu) = (\Delta_n \times \mathbb{R}, d\sigma)$  $(\Omega, \nu) = (\Delta_n \times \mathbb{R}, d\sigma)$  $(\Omega, \nu) = (\Delta_n \times \mathbb{R}, d\sigma)$ <br> $||d\sigma \times (\widehat{f^{(n)}}(t) dt)|| \le \frac{1}{n!} ||\widehat{f^{(n)}}||_1$ , the estimate [\(19\)](#page-11-2) follows.  $\blacksquare$ 

All three of the above known theorems (Theorems [3.7,](#page-10-0) [3.8,](#page-11-1) and [3.9\)](#page-11-3) are needed to prove the following new crucial result, Theorem [3.10.](#page-12-0) That theorem creates Schatten class perturbations  $\tilde{V}_j = V_j (H_j - iI)^{-1}$  out of relative Schatten class perturbations  $V_i$  inside a multiple operator integral by means of a certain change of variables. It will be used throughout this paper, in particular to apply the bound from Theorem [3.7](#page-10-0) to the relative Schatten case, in which the perturbation  $V$  is generally noncompact.

<span id="page-12-0"></span>**Theorem 3.10.** Let  $n \in \mathbb{N}$ , let  $H_0, \ldots, H_n$  be self-adjoint operators in  $\mathcal{H}$ , and let  $V_1, \ldots, V_n \in \mathcal{B}(\mathcal{H})$ . Then, the multiple operator integral given by Definition [3.6](#page-10-2) sat*isfies the following properties.*

<span id="page-12-1"></span>*i. For every*  $f \in C^n$  satisfying  $\widehat{f^{(n)}}$ ,  $\widehat{f^{(n)}}$ ,  $\widehat{f^{(n-1)}} \in L$ 1 *, we have*  $T_{f^{[n]}}^{H_0,...,H_n}(V_1,...,V_n)$  $=T_{(fu)^{[n]}}^{H_0,\dots,H_n}((H_0-iI)^{-1}V_1,V_2,\dots,V_n)$  $-(H_0 - iI)^{-1} V_1 T_{f^{[n-1]}}^{H_1,\ldots,H_n}(V_2,\ldots,V_n),$  (21)

<span id="page-12-3"></span>
$$
T_{f[n]}^{H_0, \dots, H_n}(V_1, \dots, V_n)
$$
  
=  $T_{(fu)^{[n]}}^{H_0, \dots, H_n}(V_1, \dots, \tilde{V}_j, \dots, V_n)$   
-  $T_{f^{[n-1]}}^{H_0, \dots, H_{j-1}, H_{j+1}, \dots, H_n}(V_1, \dots, \tilde{V}_j V_{j+1}, \dots, V_n)$  (22)

*for*  $j = 1, ..., n - 1$ *, and* 

<span id="page-12-2"></span>
$$
T_{f^{[n]}}^{H_0,\ldots,H_n}(V_1,\ldots,V_n)
$$
  
=  $T_{(fu)^{[n]}}^{H_0,\ldots,H_n}(V_1,\ldots,V_{n-1},\widetilde{V}_n) - T_{f^{[n-1]}}^{H_0,\ldots,H_{n-1}}(V_1,\ldots,V_{n-1})\widetilde{V}_n.$ 

ii. *Denote* 
$$
\tilde{V}_{j,l} := \tilde{V}_{j+1} \dots \tilde{V}_l
$$
. Then, for all  $f \in C_c^{n+1}$ ,  
\n
$$
T_{f^{[n]}}^{H_0, \dots, H_n}(V_1, \dots, V_n)
$$
\n
$$
= \sum_{p=0}^n \sum_{0 < j_1 < \dots < j_p \le n} (-1)^{n-p} T_{(fu^p)^{[p]}}^{H_0, H_{j_1}, \dots, H_{j_p}}(\tilde{V}_{0, j_1}, \dots, \tilde{V}_{j_{p-1}, j_p}) \tilde{V}_{j_p, n}.
$$

*If*  $V_k (H_k - iI)^{-1} \in S^n$  for all  $k = 1, ..., n$ , then the above formula holds *for every*  $f \in \mathfrak{B}_n$  *introduced in* [\(9\)](#page-8-1)*, and hence, for every*  $f \in \mathfrak{W}_n$ *.* 

<span id="page-13-3"></span>iii. If  $V_k (H_k - iI)^{-1} \in \mathcal{S}^n$  for every  $k = 1, \ldots, n$ , then

<span id="page-13-1"></span><span id="page-13-0"></span>
$$
T_{f[n]}^{H_0,...,H_n}(V_1,...,V_n) \in S^1
$$

*for every*  $f \in \mathfrak{b}_n$ *.* 

*Proof.* Since  $u^{[1]} = 1_{\mathbb{R}^2}$  and  $u^{[p]} = 0$  for all  $p \ge 2$ , the Leibniz rule for divided differences gives

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

If we swap  $\lambda_n$  with  $\lambda_j$  (for any  $j \in \{0, \ldots, n\}$ ), and rearrange using symmetry of the divided difference, we obtain

$$
f^{[n]}(\lambda_0, ..., \lambda_n) = (fu)^{[n]}(\lambda_0, ..., \lambda_n)u^{-1}(\lambda_j)
$$
  
- 
$$
f^{[n-1]}(\lambda_0, ..., \lambda_{j-1}, \lambda_{j+1}, ..., \lambda_n)u^{-1}(\lambda_j).
$$
 (23)

Applying [\(23\)](#page-13-0) repeatedly, we obtain

$$
f^{[n]}(\lambda_0, ..., \lambda_n)
$$
  
= 
$$
\sum_{p=0}^n \sum_{0 < j_1 < \dots < j_p \le n} (-1)^{n-p} (fu^p)^{[p]}(\lambda_0, \lambda_{j_1}, ..., \lambda_{j_p}) u^{-1}(\lambda_1) ... u^{-1}(\lambda_n).
$$
 (24)

Since  $\widehat{f^{(n)}}$ ,  $\widehat{(fu)^{(n)}}$ ,  $\widehat{f^{(n-1)}} \in L$ <sup>1</sup>, by Theorem [3.9,](#page-11-3) the functions  $f^{[n-1]}$  and  $(fu)^{[n]}$ admit the representation  $(18)$ . Hence, the function on the right-hand side of  $(23)$  also admits the representation [\(18\)](#page-11-0). Therefore, by Theorem [3.8](#page-11-1) applied to  $\phi = f^{[n]}$  and  $\phi$  = r.h.s of [\(23\)](#page-13-0), we obtain [\(i\)](#page-12-1). Similarly, applying Theorem [3.8](#page-11-1) and Theorem [3.9](#page-11-3) to [\(24\)](#page-13-1) gives

<span id="page-13-2"></span>
$$
T_{f_k^{[n]}}^{H_0, \dots, H_n}(V_1, \dots, V_n)
$$
  
= 
$$
\sum_{p=0}^n \sum_{0 < j_1 < \dots < j_p \le n} (-1)^{n-p} T_{(f_k u^p)^{[p]}}^{H_0, H_{j_1}, \dots, H_{j_p}}(\widetilde{V}_{0, j_1}, \dots, \widetilde{V}_{j_{p-1}, j_p}) \widetilde{V}_{j_p, n} \tag{25}
$$

for all  $f_k \in \mathfrak{b}_n$  introduced in [\(10\)](#page-8-2).

Let  $f \in \mathfrak{B}_n$ . By Lemma [3.5](#page-8-3) we can choose  $f_k \in \mathfrak{b}_n$  for all  $k \in \mathbb{N}$  such that

<span id="page-14-1"></span>
$$
\|\widehat{f_k^{(n)}} - \widehat{f^{(n)}}\|_1 \to 0 \quad \text{and} \quad \|(f_k u^p)^{(p)} - (fu^p)^{(p)}\|_{\infty} \to 0. \tag{26}
$$

The above  $L^1$ -norm-convergence implies that the left-hand side of [\(25\)](#page-13-2) converges (in operator norm) to  $T^{H_0,...,H_n}_{f^{[n]}}(V_1,...,V_n)$  by [\(19\)](#page-11-2). Moreover, we find that  $\widetilde{V}_{j_{m-1},j_m}$  $S^{\alpha_m}$ , where  $\alpha_m := n/(j_m - j_{m-1}) \in (1, \infty)$  for  $m = 2, \ldots, p$ , and  $\tilde{V}_{0,j_1} \in S^{\alpha_1}$ ,  $\widetilde{V}_{j_p,n} \in \mathcal{S}^{\alpha_p+1}$ , where  $\alpha_1 = n/j_1 \in [1,\infty), \alpha_{p+1} = n/(n-j_p) \in (1,\infty]$ . By Hölder's inequality and Theorems [3.8](#page-11-1) and [3.9,](#page-11-3) we obtain that the right-hand side of [\(25\)](#page-13-2) is in  $S<sup>1</sup>$ , implying [\(iii\)](#page-13-3). On the strength of Theorem [3.7](#page-10-0) applied to  $S<sup>2α<sub>m</sub></sup>$ , the supnormconvergence in  $(26)$  implies that the right-hand side of  $(25)$  converges to the right-hand side of [\(ii\)](#page-12-2) in the operator norm (since convergence in Schatten norms implies uniform convergence). By uniqueness of limits in  $\mathcal{B}(\mathcal{H})$ , we conclude [\(ii\)](#page-12-2).  $\blacksquare$ 

**Remark 3.11.** (i) Although the condition  $V(H - iI)^{-1} \in S^n$  is equivalent to the condition  $V(H^2 + I)^{-1/2} \in \mathcal{S}^n$ , this paper makes use of the complex weight  $u(t) =$  $t - i$  rather than the real weight  $\tilde{u}(t) = \sqrt{t^2 + 1}$ , because there is no suitable analog of Theorem [3.10](#page-12-0) for the latter. For instance, an analog of [\(23\)](#page-13-0) for  $\tilde{u}(t) := \sqrt{t^2 + 1}$ with  $n = 4$  and  $j = 1$  contains terms like

$$
f^{[2]}(\lambda_0, \lambda_2, \lambda_4) \tilde{u}^{[2]}(\lambda_1, \lambda_2, \lambda_3) u^{-1}(\lambda_1).
$$
 (27)

The latter is an obstacle to creating weights in the spirit of Theorem [3.10.](#page-12-0)

## 3.3. Taylor remainder via operator integrals

The following two results are known. We refer the interested reader to [\[21\]](#page-35-0) for additional details.

<span id="page-14-0"></span>**Theorem 3.12.** Let  $n \in \mathbb{N}$  and let  $f \in C^n$ (R) *be such that*  $\widehat{f^{(k)}} \in L^1(\mathbb{R})$ ,  $k =$ 1, ..., n. Let H be a self-adjoint operator in  $\mathcal{H}$ , let  $V \in \mathcal{B}(\mathcal{H})_{sa}$ . Then, the Fréchet derivative  $\frac{1}{k!}$  $\frac{d^{k}}{dt^{k}} f(H + tV)|_{t=0}$  exists in the operator norm and admits the multiple *operator integral representation*

<span id="page-14-2"></span>
$$
\frac{1}{k!} \frac{d^k}{ds^k} f(H + sV) \Big|_{s=t} = T_{f^{[k]}}^{H + tV, \dots, H + tV} (V, \dots, V). \tag{28}
$$

The map  $t \mapsto \frac{d^k}{ds^k} f(H + sV)|_{s=t}$  is continuous in the strong operator topology and, when  $V \in S^k$ , in the  $S^1$ -norm.

*Proof.* The first assertion is given in [\[21,](#page-35-0) Theorem 5.3.5] and, in fact, holds for a larger set of functions. The second assertion follows from [\[21,](#page-35-0) Proposition 4.3.15]. The proof relies on Theorems [3.8](#page-11-1) and [3.9.](#page-11-3)

Given a function  $f \in C^n$ (R) satisfying  $\widehat{f^{(k)}} \in L$  $\mathbf{1}(\mathbb{R}), k = 1, \ldots, n$ , a self-adjoint operator H in  $\mathcal{H}$ , and  $V \in \mathcal{B}(\mathcal{H})_{sa}$ , we denote the  $n<sup>th</sup>$  Taylor remainder by

$$
R_{n,H,f}(V) := f(H+V) - f(H) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} f(H+tV) \Big|_{t=0}.
$$
 (29)

The Taylor remainder admits the following representation in terms of a multiple operator integral.

<span id="page-15-1"></span>**Theorem 3.13.** Let  $n \in \mathbb{N}$  and let  $f \in C^n$ (R) *be such that*  $\widehat{f^{(k)}} \in L$  $^{1}(\mathbb{R}), k =$ 1, ..., *n*. Let H be a self-adjoint operator in H, let  $V \in \mathcal{B}(\mathcal{H})_{sa}$ . Then,

<span id="page-15-5"></span><span id="page-15-3"></span>
$$
R_{n,H,f}(V) = T_{f^{[n]}}^{H,H+V,H,\dots,H}(V,\dots,V),
$$
\n(30)

where  $T_{f^{[n]}}^{H,H+V,H,...,H}$  is the multilinear operator integral given by Definition [3.6](#page-10-2).

*Proof.* By [\[21,](#page-35-0) Theorem 3.3.8] for  $k = 0$  and [21, Theorem 4.3.14] for  $k \ge 1$ ,

<span id="page-15-2"></span>
$$
T_{f[k]}^{H_0, H_1 + V, H_2, \dots, H_k}(V_1, \dots, V_k) - T_{f[k]}^{H_0, \dots, H_k}(V_1, \dots, V_k)
$$
  
= 
$$
T_{f[k+1]}^{H_0, H_1 + V, H_1, \dots, H_k}(V_1, V, V_2, \dots, V_k),
$$
 (31)

where  $H_0, \ldots, H_k$  are self-adjoint operators in H and V,  $V_1, \ldots, V_k \in \mathcal{B}(\mathcal{H})_{sa}$ . In particular,

$$
T_{f^{[k]}}^{H,H+V,H,\dots,H}(V,\dots,V) - T_{f^{[k]}}^{H,\dots,H}(V,\dots,V) = T_{f^{[k+1]}}^{H,H+V,H,\dots,H}(V,\dots,V).
$$
\n(32)

Combining  $(32)$  with  $(28)$  and proceeding by induction on k yields  $(30)$ . **The Second Service** 

# 4. Existence of the spectral shift function

In this section we establish our main result.

<span id="page-15-0"></span>**Theorem 4.1.** Let  $n \in \mathbb{N}$ , let H be a self-adjoint operator in  $\mathcal{H}$ , and let  $V \in \mathcal{B}(\mathcal{H})_{sa}$ *be such that*  $V(H - iI)^{-1} \in \mathcal{S}^n$ . Then, there exists  $c_n > 0$  and a real-valued function  $\eta_n$  *such that* 

<span id="page-15-4"></span>
$$
\int_{\mathbb{R}} |\eta_n(x)| \frac{dx}{(1+|x|)^{n+\varepsilon}} \le c_n (1+\varepsilon^{-1})(1+\|V\|) \|V(H-iI)^{-1}\|_n^n \quad \text{for all } \varepsilon > 0
$$
\n(33)

*and*

<span id="page-16-1"></span>
$$
\operatorname{Tr}(R_{n,H,f}(V)) = \int_{\mathbb{R}} f^{(n)}(x) \eta_n(x) dx \tag{34}
$$

*for every*  $f \in \mathfrak{W}_n$ *. The locally integrable function*  $\eta_n$  *is determined by* [\(34\)](#page-16-1) *uniquely up to a polynomial summand of degree at most*  $n - 1$ .

We start by outlining major steps and ideas of the proof of Theorem [4.1.](#page-15-0)

In Proposition [4.2](#page-16-0) we establish a weaker version of [\(34\)](#page-16-1) with measure  $d\mu_n$  on the right-hand side of [\(34\)](#page-16-1) in place of the desired absolutely continuous measure  $\eta_n(x)$  dx. The measure  $\mu_n$ , which we call the *spectral shift measure*, satisfies the bound [\(33\)](#page-15-4). In Proposition [4.4,](#page-21-2) we establish another weaker version of [\(34\)](#page-16-1) for compactly supported f, where on the left-hand side we have a certain component of the remainder and on the right-hand side in place of  $f$  we have its product with some complex weight. By combining advantages of the results of Propositions [4.2](#page-16-0) and [4.4,](#page-21-2) we derive the trace formula [\(34\)](#page-16-1).

One of our main tools is multilinear operator integration developed for Schatten class perturbations. We have onset technical obstacles since our perturbations are not compact. To bridge the gap between existing results and our setting we impose suitable weights on the perturbations and involve multistage approximation arguments. In particular, the proof of Proposition [4.4](#page-21-2) requires two novel techniques. The first one is a new expression for the remainder  $R_{n,H,f}(V)$  in terms of handy components that are continuous in  $V$  in a very strong sense. The second one is an approximation argument that allows replacing relative Schatten  $V$  by finite rank  $V_k$  and strengthens convergence arguments present in the literature.

### <span id="page-16-3"></span>4.1. Existence of the spectral shift measure

The following result is our first major step in the proof of the representation [\(34\)](#page-16-1).

<span id="page-16-0"></span>**Proposition 4.2.** Let  $n \in \mathbb{N}$ , let H be a self-adjoint operator in  $\mathcal{H}$ , and let  $V \in$  $\mathcal{B}(\mathcal{H})_{sa}$  *be such that*  $V(H - iI)^{-1} \in \mathcal{S}^n$ . Then, there exists a Borel measure  $\mu_n$  such *that*

<span id="page-16-4"></span><span id="page-16-2"></span>
$$
\operatorname{Tr}(R_{n,H,f}(V)) = \int_{\mathbb{R}} f^{(n)} d\mu_n \tag{35}
$$

*for every*  $f \in \mathfrak{W}_n$  *and* 

$$
d\mu_n(x) = u^n(x) \, dv_n(x) + \xi_n(x) \, dx,\tag{36}
$$

*where*  $v_n$  *is a finite measure satisfying* 

<span id="page-17-2"></span><span id="page-17-1"></span>
$$
||v_n|| \le c_n (1 + ||V||) ||V(H - iI)^{-1}||_n^n,
$$
\n(37)

*and*  $\xi_n$  *is a continuous function satisfying* 

$$
|\xi_n(x)| \le c_n (1 + \|V\|) \|V(H - iI)^{-1}\|_n^n (1 + |x|)^{n-1}, \quad x \in \mathbb{R},\tag{38}
$$

*for some constant*  $c_n > 0$ . If  $\tilde{\mu}_n$  *is another locally finite Borel measure such that* [\(35\)](#page-16-2) *holds for all*  $f \in C_c^{n+1}$ *, then*  $d\tilde{\mu}_n(x) = d\mu_n(x) + p_{n-1}(x) dx$ *, where*  $p_{n-1}$  *is a polynomial of degree at most*  $n - 1$ *.* 

To prove Proposition [4.2](#page-16-0) we need the estimate stated below.

<span id="page-17-0"></span>**Lemma 4.3.** *Let*  $k \in \mathbb{N}$ , *let*  $H_0, \ldots, H_k$  *be self-adjoint operators in*  $\mathcal{H}$ , *let*  $\alpha_1 \ldots, \alpha_k \in$  $(1, \infty)$  be such that  $\frac{1}{\alpha_1} + \cdots + \frac{1}{\alpha_k} = 1$ , and let  $B_j \in S^{\alpha_k}$ ,  $j = 1, \ldots, k$ . Then, there *exists*  $c_{\alpha} := c_{\alpha_1,\dots,\alpha_k} > 0$  *such that for multiple operator integrals given by Definition* [3.6](#page-10-2)*,*

$$
|\operatorname{Tr}(T_{f^{[k]}}^{H_k, H_1, ..., H_k}(B_1, ..., B_k))| \le c_{\alpha} \|f^{(k)}\|_{\infty} \|B_1\|_{\alpha_1} ... \|B_k\|_{\alpha_k} \quad (\widehat{f^{(k)}} \in L^1)
$$

*and*

$$
|\operatorname{Tr}(B_1 T_{f[k-1]}^{H_0,\ldots,H_{k-1}}(B_2,\ldots,B_k))|
$$
  
 
$$
\leq c_{\alpha} \|f^{(k-1)}\|_{\infty} \|B_1\|_{\alpha_1} \ldots \|B_k\|_{\alpha_k} \quad (f \in C_b^{k-1}).
$$

*Consequently, there exist unique (complex) Borel measures*  $\mu_1, \mu_2$  with total variation *bounded by*  $c_{\alpha}$  ||  $B_1$  ||  $_{\alpha_1}$  . . . ||  $B_k$  ||  $_{\alpha_k}$  such that

$$
\text{Tr}(T_{f^{[k]}}^{H_k, H_1, \dots, H_k}(B_1, \dots, B_k)) = \int\limits_{\mathbb{R}} f^{(k)} d\mu_1 \quad (\widehat{f^{(k)}} \in L^1)
$$

*and*

$$
\operatorname{Tr}(B_1 T_{f^{[k-1]}}^{H_0,\ldots,H_{k-1}}(B_2,\ldots,B_k)) = \int\limits_{\mathbb{R}} f^{(k-1)} d\mu_2 \quad (f \in C_0^{k-1}).
$$

*Proof.* The first assertion follows from [\[14,](#page-34-5) Theorem 5.3 and Remark 5.4], Hölder's inequality, and [\[21,](#page-35-0) Theorem 4.3.10]. The second assertion is subsequently obtained by the Riesz–Markov representation theorem for a bounded linear functional on the space  $C_0(\mathbb{R})$ .

*Proof of Proposition* [4.2](#page-16-0). Let  $n \ge 2$ . Using [\(30\)](#page-15-3) and Theorem [3.10](#page-12-0) [\(ii\)](#page-12-2), we obtain

$$
R_{n,H,f}(V) = T_{f^{[n]}}^{H,H+V,H,...,H}(V,...,V)
$$
  
= 
$$
\sum_{p=0}^{n} \sum_{\substack{j_1,...,j_p \ge 1, j_{p+1} \ge 0 \\ j_1 + \cdots + j_{p+1} = n}} (-1)^{n-p} T_{(fu^p)^{[p]}}^{H,H_{j_1},H,...,H}(\tilde{V}^{j_1}, ..., \tilde{V}^{j_p}) \tilde{V}^{j_{p+1}},
$$
 (39)

where  $H_1 = H + V$  and  $H_{j_1} = H$  for  $j_1 \neq 1$ , and in which the first factor of  $\tilde{V}$  in the first input of the multilinear operator integral should be interpreted as  $V(H + V (iI)^{-1}$ . By the second resolvent identity,

<span id="page-18-0"></span>
$$
||V(H + V - iI)^{-1}||_{n} \le (1 + ||V||) ||V(H - iI)^{-1}||_{n}.
$$
 (40)

By the definition of  $\mathfrak{W}_n$  (see Definition [3.1\)](#page-7-0) and property [\(8\)](#page-7-4), we obtain  $(fu^p)^{(p)} \in$  $C_0(\mathbb{R})$  for every  $f \in \mathfrak{W}_n$ ,  $p = 0, \ldots, n$ . Hence, by Lemma [4.3](#page-17-0) applied to each term of [\(39\)](#page-18-0), there exist unique Borel measures  $\mu_0, \ldots, \mu_n$  such that

$$
\|\check{\mu}_P\| \le C_n (1 + \|V\|) \|V(H - iI)^{-1}\|_n^n \tag{41}
$$

and

<span id="page-18-1"></span>
$$
\text{Tr}(R_{n,H,f}(V)) = \sum_{p=0}^{n} \int (fu^p)^{(p)} d\mu_p \tag{42}
$$

for every  $f \in \mathfrak{W}_n, n \geq 2$ .

Let  $n = 1$ . By Theorem [3.12](#page-14-0) and the fundamental theorem of calculus,

$$
R_{1,H,f}(V) = f(H+V) - f(H) = \int_{0}^{1} T_{f^{[1]}}^{H_t, H_t}(V) dt
$$

for  $f \in \mathfrak{W}_1$ , where  $H_t = H + tV$ . By [\(22\)](#page-12-3) of Theorem [3.10](#page-12-0) [\(i\)](#page-12-1) for  $j = 1$  applied to  $T_{f[1]}^{H_t, H_t}(V)$  and by continuity of the trace, we obtain

$$
\operatorname{Tr}(R_{1,H,f}(V)) = \int_{0}^{1} \operatorname{Tr}(T_{(fu)^{[1]}}^{H_t, H_t}(V(H_t - iI)^{-1}) - f(H_t)V(H_t - iI)^{-1}) dt.
$$

Noticing that

$$
\sup_{t \in [0,1]} \|V(H_t - iI)^{-1}\|_1 \le (1 + \|V\|) \|V(H - iI)^{-1}\|_1,
$$

using the property of the double operator integral  $\text{Tr}(T_{g^{[1]}}^{H,H}(V)) = \text{Tr}(g'(H)V)$ , and applying Hölder's inequality and the Riesz–Markov representation theorem completes the proof of [\(42\)](#page-18-1) for  $n = 1$ .

Let  $n \in \mathbb{N}$ . Applying a higher order differentiation product rule on the right-hand side of [\(42\)](#page-18-1) gives

$$
\text{Tr}(R_{n,H,f}(V)) = \sum_{p=0}^{n} \sum_{k=0}^{p} {p \choose k} \frac{p!}{k!} \int f^{(k)} u^k d\mu_p
$$

$$
= \sum_{k=0}^{n-1} \int f^{(k)} u^k d\mu_k + \int f^{(n)} u^n d\nu_n, \tag{43}
$$

for some Borel measures  $\hat{\mu}_0, \dots, \hat{\mu}_{n-1}, \nu_n$  satisfying

$$
\|\dot{\mu}_0\|, \ldots, \|\dot{\mu}_{n-1}\|, \|v_n\| \le \widetilde{C}_n (1 + \|V\|) \|V(H - iI)^{-1}\|_n^n. \tag{44}
$$

Integrating by parts in [\(43\)](#page-19-0) and applying

<span id="page-19-2"></span><span id="page-19-0"></span>
$$
\lim_{x \to \pm \infty} f^{(k)}(x) u^k(x) = 0, \quad k = 0, \dots, n - 1,
$$
\n(45)

(see [\(8\)](#page-7-4) in the proof of Proposition [3.3\)](#page-7-1) yields

$$
\text{Tr}(R_{n,H,f}(V)) = -\sum_{k=0}^{n-1} \int_{-\infty}^{\infty} (f^{(k+1)}u^k + kf^{(k)}u^{k-1})(x)\dot{\mu}_k((-\infty, x)) dx
$$

$$
+ \int f^{(n)}u^n \, dv_n.
$$

Since

<span id="page-19-1"></span>
$$
f^{(k)}u^{k-1} \in L^1(\mathbb{R}), \quad k = 1, ..., n,
$$

we rearrange the terms above to obtain

$$
\text{Tr}(R_{n,H,f}(V)) = \sum_{k=1}^{n} \int f^{(k)}(x)u^{k-1}(x)\tilde{\xi}_k(x) dx + \int f^{(n)}u^n dv_n, \qquad (46)
$$

where  $\tilde{\xi}_k$  are continuous functions defined by

$$
\tilde{\xi}_k(x) = -\hat{\mu}_{k-1}((-\infty, x)) - k\hat{\mu}_k((-\infty, x)), \quad k = 1, ..., n-1,
$$
  
\n
$$
\tilde{\xi}_n(x) = -\hat{\mu}_{n-1}((-\infty, x)),
$$

so that

<span id="page-19-3"></span>
$$
\|\tilde{\xi}_k\|_{\infty} \le c_{n,k}(1 + \|V\|) \|V(H - iI)^{-1}\|_{n}^{n}, \quad k = 1, \dots, n. \tag{47}
$$

By a repeated partial integration in  $(46)$  and application of  $(45)$ , we obtain

$$
\operatorname{Tr}(R_{n,H,f}(V)) = \int_{\mathbb{R}} f^{(n)} d\mu_n \quad (f \in \mathfrak{W}_n)
$$

with

<span id="page-20-0"></span>
$$
d\mu_n(x) = u^n(x) dv_n(x) + \xi_n(x) dx,
$$
\n(48)

where

$$
\xi_n(s_0) := \sum_{k=1}^n (-1)^{n-k} \int_0^{s_0} ds_1 \cdots \int_0^{s_{n-k-1}} u^{k-1}(s_{n-k}) \tilde{\xi}_k(s_{n-k}) ds_{n-k}.
$$
 (49)

The function  $\xi_n$  given by [\(49\)](#page-20-0) is continuous. To confirm [\(38\)](#page-17-1) we note that, for all  $m \in \mathbb{N}$ ,

$$
\sup_{x \in \mathbb{R}} \left| u^{-m}(x) \int_{0}^{x} g(t) dt \right| \leq \sup_{x \in \mathbb{R}} \left( \left| \frac{x}{u(x)} \right| \sup_{|t| \leq |x|} |u^{1-m}(x)g(t)| \right) \leq \| u^{1-m} g \|_{\infty}.
$$
 (50)

By applying [\(50\)](#page-20-1)  $(n - k)$ -times in [\(49\)](#page-20-0) and using the bound [\(47\)](#page-19-3), we obtain

$$
|\xi_n(x)| \le c_n (1 + \|V\|) \|V(H - iI)^{-1}\|_n^n (1 + |x|)^{n-1}, \quad x \in \mathbb{R}.\tag{51}
$$

We have thereby proven the first part of the proposition.

To prove the second part of the proposition, we let  $\tilde{\mu}_n$  be a locally finite measure such that [\(35\)](#page-16-2) holds for all  $f \in C_c^{n+1}$  and denote

<span id="page-20-2"></span><span id="page-20-1"></span>
$$
\rho_n:=\mu_n-\tilde{\mu}_n.
$$

Then,

$$
\int f^{(n)} d\rho_n = 0 \quad (f \in C_c^{n+1}).
$$
\n(52)

We are left to confirm that

$$
d\rho_n(x) = p_{n-1}(x) dx, \qquad (53)
$$

where  $p_{n-1}$  is a polynomial of degree at most  $n - 1$ . Consider the distribution T defined by

<span id="page-20-3"></span>
$$
T(g):=\int g\ d\rho_n
$$

for all  $g \in C_c^{\infty}(\mathbb{R})$ . By [\(52\)](#page-20-2) and the definition of the derivative of a distribution,  $T^{(n)} = 0$ . Since the primitive of a distribution is unique up to an additive constant (see, e.g.,  $[1,$  Theorem 3.10]), by an inductive argument (see, e.g.,  $[1,$  Example 2.21]), we obtain  $(53)$ .  $\blacksquare$ 

#### 4.2. Alternative trace formula

The following result is our second major step in the proof of the representation [\(34\)](#page-16-1). It provides an alternative to [\(34\)](#page-16-1) with weighted  $f$  on the right-hand side. It also provides an alternative to  $(35)$  with weighted f on the right-hand side, thereby effectively replacing the measure  $\mu_n$  with functions  $\breve{\eta}_0, \ldots, \breve{\eta}_{n-1} \in L^1_{loc}$ .

<span id="page-21-2"></span>**Proposition 4.4.** Let  $n \in \mathbb{N}$ ,  $n \geq 3$ , let H be a self-adjoint operator in H, and let  $V \in \mathcal{B}(\mathcal{H})_{sa}$  *satisfy*  $V(H - iI)^{-1} \in \mathcal{S}^n$ . Then, for every  $p = 0, \ldots, n - 1$ , there exists  $\breve{\eta}_p \in L^1_{\text{loc}}$  such that

$$
\operatorname{Tr}(R_{n,H,f}(V)) = \sum_{p=0}^{n-1} (-1)^{n-1-p} \int_{\mathbb{R}} (fu^p)^{(p+1)}(x) \check{\eta}_p(x) dx \tag{54}
$$

*for all*  $f \in C_c^{n+1}$ .

In order to prove [\(54\)](#page-21-3), firstly we decompose  $R_{n,H,f}(V)$  into more convenient components for which we can derive trace formulas by utilizing the method of Section [4.1,](#page-16-3) partial integration, and approximation arguments.

<span id="page-21-1"></span>**Lemma 4.5.** Let H be a self-adjoint operator in H, let  $V \in \mathcal{B}(\mathcal{H})_{sa}$ , let  $n \in \mathbb{N}$ , and  $let f \in C_c^{n+1}$ *. Then,* 

<span id="page-21-4"></span><span id="page-21-3"></span><span id="page-21-0"></span>
$$
R_{n,H,f}(V) = \sum_{p=0}^{n-1} (-1)^{n-1-p} \widetilde{R}_{n,H,f}^p(V),
$$

*where*

$$
\widetilde{R}_{1,H,f}^{0}(V) := f(H+V) - f(H),
$$
\n
$$
\widetilde{R}_{n,H,f}^{0}(V) := f(H)V((H+V-iI)^{-1} - (H-iI)^{-1})\widetilde{V}^{n-2}
$$
\n(55)

*for*  $n \geq 2$  *and* 

$$
\widetilde{R}_{n,H,f}^{p}(V)
$$
\n
$$
:= \sum_{\substack{j_1,\dots,j_p \ge 1, j_{p+1} \ge 0 \\ j_1 + \dots + j_{p+1} = n-1}} \left( T_{(fu^p)^{[p]}}^{H,H_{j_1},H,\dots,H} (V(H + V - iI)^{-1} \widetilde{V}^{j_1-1}, \dots, \widetilde{V}^{j_p}) \widetilde{V}^{j_{p+1}} - T_{(fu^p)^{[p]}}^{H,\dots,H} (\widetilde{V}^{j_1}, \dots, \widetilde{V}^{j_p}) \widetilde{V}^{j_{p+1}} \right)
$$
\n(56)

*for*  $p = 1, ..., n - 1$ *, with*  $H_1 = H + V$  *and*  $H_{j_1} = H$  *for*  $j_1 \neq 1$ *.* 

<span id="page-22-1"></span><span id="page-22-0"></span> $\blacksquare$ 

*Proof.* Using [\(28\)](#page-14-2) and [\(30\)](#page-15-3), we get

$$
R_{n,H,f}(V) = R_{n-1,H,f}(V) - \frac{1}{(n-1)!} \frac{d^{n-1}}{dt^{n-1}} f(H + tV) \Big|_{t=0}
$$
  
=  $T_{f[n-1]}^{H,H+V,H,...,H}(V,...,V) - T_{f[n-1]}^{H,...,H}(V,...,V).$  (57)

An application of Theorem [3.10](#page-12-0) [\(ii\)](#page-12-2) to each of the terms in [\(57\)](#page-22-0) completes the proof.

Firstly, we show that  $(54)$  holds when V is a finite-rank operator. This is done by establishing an analog of [\(54\)](#page-21-3) for  $\tilde{R}_{n,H,f}^p(V)$  and then extending (54) to  $R_{n,H,f}(V)$ with help of Lemma [4.5.](#page-21-1)

<span id="page-22-2"></span>**Proposition 4.6.** Let  $n \in \mathbb{N}$ ,  $n \geq 3$ , let H be a self-adjoint operator in H, and let  $V \in \mathcal{B}(\mathcal{H})_{sa}$  *be of finite rank. Then, for*  $p = 0, \ldots, n - 1$ *, there exists*  $\breve{\eta}_p \in L^1_{loc}$  *such that*

$$
\operatorname{Tr}(\widetilde{R}_{n,H,f}^p(V)) = \int_{\mathbb{R}} (fu^p)^{(p+1)}(x)\check{\eta}_p(x) dx
$$

for all  $f \in C_c^{n+1}$ , where  $\widetilde{R}_{n,H,f}^p$  is given by [\(56\)](#page-21-0).

*Proof.* By the definition of  $\widetilde{R}_{n,H,f}^p(V)$  in Lemma [4.5,](#page-21-1)

$$
|\operatorname{Tr}(\widetilde{R}_{n,H,f}^{p}(V))|
$$
  
\n
$$
\leq \sum_{\substack{j_1,\ldots,j_p\geq 1,j_{p+1}\geq 0\\j_1+\cdots+j_{p+1}=n-1}} (|\operatorname{Tr}(T_{(fu^p)^{[p]}}^{H,H_{j_1},H,\ldots,H}(V(H+V-iI)^{-1}\widetilde{V}^{j_1-1},\ldots,\widetilde{V}^{j_p})\widetilde{V}^{j_{p+1}})| + |\operatorname{Tr}(T_{(fu^p)^{[p]}}^{H,\ldots,H}(\widetilde{V}^{j_1},\ldots,\widetilde{V}^{j_p})\widetilde{V}^{j_{p+1}})|). \tag{58}
$$

By Lemma [4.3](#page-17-0) applied to each summand on the right-hand side of [\(58\)](#page-22-1),

$$
|\operatorname{Tr}(\widetilde{R}_{n,H,f}^{p}(V))|
$$
  
\n
$$
\leq \sum_{\substack{j_1,\ldots,j_p\geq 1, j_{p+1}\geq 0\\j_1+\cdots+j_{p+1}=n-1}} 2c_{n,j} \|(fu^p)^{(p)}\|_{\infty} (1+\|V\|) \|V(H-iI)^{-1}\|_{n-1}^{n-1}
$$
  
\n
$$
=: c_n \|(fu^p)^{(p)}\|_{\infty} (1+\|V\|) \|V(H-iI)^{-1}\|_{n-1}^{n-1}.
$$
 (59)

Hence, by the Riesz–Markov representation theorem, there exist unique Borel measures  $\mu_p$  such that

$$
\|\check{\mu}_p\| \le c_n (1 + \|V\|) \|V(H - iI)^{-1}\|_{n-1}^{n-1}
$$

and

$$
\operatorname{Tr}(\widetilde{R}_{n,H,f}^p(V)) = \int (fu^p)^{(p)} d\mathring{\mu}_p
$$

for all  $f \in C_c^{n+1} \subseteq \mathfrak{W}_n$ . Hence,  $\eta_p(x) := -\mu_p((-\infty, x))$  is a bounded function in  $L^1_{loc}(\mathbb{R})$  and the proposition follows by the partial integration formula for distribution functions.

Proposition [4.6](#page-22-2) will be extended from finite rank to relative Schatten class perturbations by an approximation argument. To carry out the latter we build some technical machinery below.

We need the next standard result in operator theory.

<span id="page-23-2"></span>**Lemma 4.7.** *Let*  $\alpha, \alpha_j \in [1, \infty]$  *satisfy*  $\frac{1}{\alpha_1} + \cdots + \frac{1}{\alpha_n} = \frac{1}{\alpha}$ *. Denote*  $\mathcal{L}^{\alpha} := (\mathcal{S}^{\alpha}, ||\cdot||_{\alpha})$ *for*  $\alpha \in [1, \infty)$  and  $\mathcal{L}^{\infty} := (\mathcal{B}(\mathcal{H})_1, \text{so}^*)$ , where  $\mathcal{B}(\mathcal{H})_1$  denotes the closed unit ball  $in \mathcal{B(H)}$ *. Then, the function* 

$$
(A_1,\ldots,A_n)\mapsto A_1\ldots A_n
$$

*is a continuous map from*  $\mathcal{L}^{\alpha_1} \times \cdots \times \mathcal{L}^{\alpha_n}$  to  $\mathcal{L}^{\alpha}$ .

The following approximation of weighted perturbations is an important step in the approximation of the trace formula given by Proposition [4.6.](#page-22-2)

<span id="page-23-0"></span>Lemma 4.8. *Let* H *be a Hilbert space,* H *a self-adjoint operator in* H*, and let*  $V \in \mathcal{B}(\mathcal{H})_{sa}$  *be such that*  $V(H - iI)^{-1} \in \mathcal{S}^n$ . Then, there exists a sequence  $(V_k)_k \subset$  $\mathcal{B}(\mathcal{H})_{sa}$  *of finite-rank operators such that*  $(V_k)_k$  *converges strongly to* V *and such that*

$$
||V_k(H - iI)^{-1} - V(H - iI)^{-1}||_n \to 0 \quad \text{as } k \to \infty \tag{60}
$$

*and, moreover,*

$$
||V_k|| \le ||V|| \quad \text{and} \quad ||V_k(H - iI)^{-1}||_n \le ||V(H - iI)^{-1}||_n. \tag{61}
$$

*Proof.* We start with a sequence of spectral projections, denoted

<span id="page-23-3"></span><span id="page-23-1"></span>
$$
P_k := E_H((-k,k)),
$$

which by the functional calculus converges strongly to  $I$ . Applying subsequently the property of orthogonal projections and standard functional calculus we obtain

$$
(P_k VP_k)((H - iI)^{-1}P_k + (I - P_k)) = (P_k VP_k)((H - iI)^{-1}P_k)
$$
  
=  $P_k V(H - iI)^{-1}P_k \in \mathcal{S}^n$  (62)

for each  $k \in \mathbb{N}$ . By the functional calculus,  $(H - iI)^{-1}P_k + (I - P_k)$  is invertible. Therefore, from [\(62\)](#page-23-1) we derive

$$
P_k V P_k = P_k V (H - iI)^{-1} P_k ((H - iI)^{-1} P_k + (I - P_k))^{-1} \in \mathcal{S}^n.
$$

For a fixed  $k$ , by the spectral theorem of compact self-adjoint operators, there exists a sequence  $(E_l)_{l=1}^{\infty}$  of finite-rank projections, each  $E_l$  commuting with  $P_k VP_k$ , such that  $E_l P_k VP_k$  converges to  $P_k VP_k$  in  $S^n$  as  $l \to \infty$ . For all  $k \in \mathbb{N}$ , there exists  $l_k \in \mathbb{N}$ such that

$$
||E_{l_k} P_k VP_k - P_k VP_k||_n < 1/k.
$$

Define

$$
V_k := E_{l_k} P_k V P_k.
$$

Then  $||V_k|| \le ||V||$  holds,  $V_k$  is self-adjoint,  $V_k \to V$  strongly, and

$$
||V_k(H - iI)^{-1} - V(H - iI)^{-1}||_n
$$
  
\n
$$
\leq ||E_{l_k} P_k V P_k - P_k V P_k||_n ||(H - iI)^{-1}||_n
$$
  
\n
$$
+ ||P_k V (H - iI)^{-1} P_k - V(H - iI)^{-1}||_n.
$$

By Lemma [4.7,](#page-23-2) the latter expression converges to 0 as  $k \to \infty$ . The second inequality in [\(61\)](#page-23-3) follows from the estimate

$$
||E_{l_k} P_k V P_k (H - iI)^{-1}||_n \le ||E_{l_k}|| ||P_k|| ||V (H - iI)^{-1}||_n ||P_k||.
$$

Our approximation on the left-hand side of the trace formula in Proposition [4.6](#page-22-2) is based on the next estimate.

<span id="page-24-0"></span>**Lemma 4.9.** Let H be a self-adjoint operator in  $\mathcal{H}$ , let  $n \in \mathbb{N}$ ,  $n \neq 2$ , and let  $V \in \mathcal{B}(\mathcal{H})_{sa}$  *be such that*  $V(H - iI)^{-1} \in \mathcal{S}^n$ . Let  $(V_k)_k \subset \mathcal{B}(\mathcal{H})_{sa}$  *be a sequence satisfying the assertions of Lemma* [4.8](#page-23-0)*. Let*  $W \in \{V, V_m\}$ *, where*  $m \in \mathbb{N}$ *. Then, given*  $a > 0$ , there exists  $c_{n,H,V,a} > 0$  such that

$$
|\operatorname{Tr}(\widetilde{R}_{n,H,f}^p(V_k)-\widetilde{R}_{n,H,f}^p(W))|\leq c_{n,H,V,a}||(fu^p)^{(p+1)}\|_{\infty}\|\widetilde{V}_k-\widetilde{W}\|_n
$$

*for all*  $p = 0, \ldots, n - 1, k \in \mathbb{N}$ , and  $f \in C_c^{n+1}[-a, a]$ , where  $\widetilde{R}_{n,H,f}^p$  *is given by* [\(56\)](#page-21-0).

*Proof.* Let  $n \geq 3$ . By [\(56\)](#page-21-0) in Lemma [4.5,](#page-21-1)

<span id="page-24-1"></span>
$$
\widetilde{R}_{n,H,f}^{p}(V_{k}) - \widetilde{R}_{n,H,f}^{p}(W)
$$
\n
$$
= \sum_{\substack{j_1,\ldots,j_p \ge 1, j_{p+1} \ge 0 \\ j_1 + \cdots + j_{p+1} = n-1}} \left( T_{(fu^p)^{[p]}}^{H,H+V_{k,j_1},H,\ldots,H} (V_{k}(H+V_{k}-iI)^{-1} \widetilde{V}_{k}^{j_1-1}, \ldots, \widetilde{V}_{k}^{j_p}) \widetilde{V}_{k}^{j_{p+1}}
$$
\n
$$
- T_{(fu^p)^{[p]}}^{H,H+W_{j_1},H,\ldots,H} (W(H+W-iI)^{-1} \widetilde{W}^{j_1-1}, \ldots, \widetilde{W}^{j_p}) \widetilde{W}^{j_{p+1}}
$$
\n
$$
- T_{(fu^p)^{[p]}}^{H,\ldots,H} (\widetilde{V}_{k}^{j_1}, \ldots, \widetilde{V}_{k}^{j_p}) \widetilde{V}_{k}^{j_{p+1}} + T_{(fu^p)^{[p]}}^{H,\ldots,H} (\widetilde{W}^{j_1}, \ldots, \widetilde{W}^{j_p}) \widetilde{W}^{j_{p+1}}), \tag{63}
$$

where  $V_{k,1} = V_k$ ,  $W_1 = W$  and  $V_{k,j} = W_j = 0$  for  $j \neq 1$ . Below we also use the notations  $\tilde{V}_k^j = V_k (H + V_k - iI)^{-1} \tilde{V}_k^{j-1}$  $\tilde{W}_{k}^{j-1}$  and  $\tilde{W}^{j} = W(H + W - iI)^{-1}\tilde{W}^{j-1}$ . By [\(31\)](#page-15-5), for  $p \ge 1$  we have

$$
T_{(fu^p)^{[p]}}^{H, H+V_k, H, \dots, H} (\tilde{V}_k^{j_1}, \dots, \tilde{V}_k^{j_p}) \tilde{V}_k^{j_{p+1}}
$$
  
=  $T_{(fu^p)^{[p+1]}}^{H, H+V_k, H+W, H, \dots, H} (\tilde{V}_k^{j_1}, V_k - W, \tilde{V}_k^{j_2}, \dots, \tilde{V}_k^{j_p}) \tilde{V}_k^{j_{p+1}}$   
+  $T_{(fu^p)^{[p]}}^{H, H+W, H, \dots, H} (\tilde{V}_k^{j_1}, \dots, \tilde{V}_k^{j_p}) \tilde{V}_k^{j_{p+1}}.$  (64)

By telescoping and [\(31\)](#page-15-5) for  $p \ge 1$  we obtain

$$
T_{(f u^p)^{[p]}}^{H, H+W, H, ..., H}(\tilde{V}_k^{j_1}, \dots, \tilde{V}_k^{j_p}) \tilde{V}_k^{j_{p+1}} - T_{(f u^p)^{[p]}}^{H, H+W, H, ..., H}(\tilde{W}^{j_1}, \dots, \tilde{W}^{j_p}) \tilde{W}^{j_{p+1}} - T_{(f u^p)^{[p]}}^{H, ..., H}(\tilde{V}_k^{j_1}, \dots, \tilde{V}_k^{j_p}) \tilde{V}_k^{j_{p+1}} + T_{(f u^p)^{[p]}}^{H, ..., H}(\tilde{W}^{j_1}, \dots, \tilde{W}^{j_p}) \tilde{W}^{j_{p+1}} = \sum_{l=1}^{p+1} (T_{(f u^p)^{[p]}}^{H, H+W, H, ..., H} - T_{(f u^p)^{[p]}}^{H, ..., H}) \times (\tilde{V}_k^{j_1}, \dots, \tilde{V}_k^{j_{l-1}}, \tilde{V}_k^{j_l} - \tilde{W}^{j_l}, \tilde{W}^{j_{l+1}}, \dots, \tilde{W}^{j_p}) \tilde{W}^{j_{p+1}} = \sum_{l=1}^{p+1} T_{(f u^p)^{[p+1]}}^{H, H+W, H, ..., H}(\tilde{V}_k^{j_1}, W, \tilde{V}_k^{j_2}, \dots, \tilde{V}_k^{j_{l-1}}, \tilde{V}_k^{j_l} - \tilde{W}^{j_l},
$$
\n
$$
\tilde{W}^{j_{l+1}}, \dots, \tilde{W}^{j_p}) \tilde{W}^{j_{p+1}}.
$$
\n(65)

<span id="page-25-0"></span>Combining [\(63\)](#page-24-1)–[\(65\)](#page-25-0) and [\(22\)](#page-12-3) of Theorem [3.10](#page-12-0) [\(i\)](#page-12-1) and adjusting the argument to the terms with  $V_k$  yields

$$
\tilde{R}_{n,H,f}^{p}(V_{k}) - \tilde{R}_{n,H,f}^{p}(W)
$$
\n
$$
= \sum_{\substack{j_{1},...,j_{p}\geq 1,j_{p+1}\geq 0\\j_{1}+\cdots+j_{p+1}=n-1}} (T_{(fu^{p+1})[p+1]}^{H,H+V_{k,j_{1}},H+W_{j_{1}},H,\ldots,H}(\check{V}_{k}^{j_{1}},(V_{k,j_{1}}-W_{j_{1}})(H+W-iI)^{-1},
$$
\n
$$
\tilde{V}_{k}^{j_{2}},\ldots,\tilde{V}_{k}^{j_{p}})\tilde{V}_{k}^{j_{p+1}}
$$
\n
$$
-T_{(fu^{p})[p]}^{H,H+V_{k,j_{1}},H,\ldots,H}(\check{V}_{k}^{j_{1}},(V_{k,j_{1}}-W_{j_{1}})(H+W-iI)^{-1}\tilde{V}_{k}^{j_{2}},\ldots,\tilde{V}_{k}^{j_{p}})\tilde{V}_{k}^{j_{p+1}}
$$
\n
$$
+\sum_{l=1}^{p+1} (T_{(fu^{p+1})[p+1]}^{H,H+W_{j_{1}},H,\ldots,H}(\tilde{V}_{k}^{j_{1}},\tilde{W}_{j_{1}},\tilde{V}_{k}^{j_{2}},\ldots,\tilde{V}_{k}^{j_{l-1}},\tilde{V}_{k}^{j_{l}}-\tilde{W}^{j_{l}},
$$
\n
$$
\tilde{W}^{j_{l+1}},\ldots,\tilde{W}^{j_{p}})\tilde{W}^{j_{p+1}}
$$
\n
$$
-T_{(fu^{p})[p]}^{H,H+W_{j_{1}},H,\ldots,H}(\tilde{V}_{k}^{j_{1}},\tilde{W}_{j_{1}}\tilde{V}_{k}^{j_{2}},\ldots,\tilde{V}_{k}^{j_{l-1}},\tilde{V}_{k}^{j_{l}}-\tilde{W}^{j_{l}},
$$
\n
$$
\tilde{W}^{j_{l+1}},\ldots,\tilde{W}^{j_{p}})\tilde{W}^{j_{p+1}}
$$
\n
$$
-T_{(fu^{p})[p]}^{H,H+W_{j_{1}},H,\ldots,H}(\check{V}_{k}^{j_{1}+1},\tilde{V}_{k}^{j_{2}},\ldots,\tilde{V}_{k}^{j_{l-1}},\til
$$

<span id="page-25-1"></span>A straightforward application of the second resolvent identity implies

$$
(V_k - W)(H + W - iI)^{-1} = (V_k - W)(H - iI)^{-1}(I - W(H + W - iI)^{-1}).
$$

For each  $W \in \{V, V_m\}$ , by the estimates [\(61\)](#page-23-3) of Lemma [4.8,](#page-23-0) we obtain

<span id="page-26-0"></span>
$$
\|\widetilde{W}\|_n \le \|\widetilde{V}\|_n. \tag{67}
$$

and

$$
||I - W(H + W - iI)^{-1}|| \le 1 + ||V||.
$$

By the latter estimate,

$$
|| (V_k - W)(H + W - iI)^{-1} ||_n \leq (1 + ||V||) ||\widetilde{V}_k - \widetilde{W}||_n.
$$

It follows from [\(67\)](#page-26-0) and the telescoping identity

$$
\widetilde{V}_k^j - \widetilde{W}^j = \sum_{i=0}^{j-1} \widetilde{V}_k^i (\widetilde{V}_k - \widetilde{W}) \widetilde{W}^{j-1-i}
$$

that

$$
\|\widetilde{V}_k^j - \widetilde{W}^j\|_{n/j} \leq j \|\widetilde{V}\|_n^{j-1} \|\widetilde{V}_k - \widetilde{W}\|_n.
$$

Applying the latter bound and Lemma [4.3](#page-17-0) in [\(66\)](#page-25-1) implies

$$
|\operatorname{Tr}(\widetilde{R}_{n,H,f}^{p}(V_{k}) - \widetilde{R}_{n,H,f}^{p}(W))|
$$
  
\n
$$
\leq \sum_{\substack{j_1,\ldots,j_p \geq 1, j_{p+1} \geq 0 \\ j_1 + \cdots + j_{p+1} = n-1}} (c_{n,j}^{1} \| (fu^{p+1})^{(p+1)} \|_{\infty} + c_{n,j}^{2} \| (fu^{p})^{(p)} \|_{\infty} ) C_{n,V,H} \| \widetilde{V}_{k} - \widetilde{W} \|_{n},
$$
\n(68)

for some constants  $c_{n,j}^1$  and  $c_{n,j}^2$  depending only on n and  $j_1, \ldots, j_{p+1}$ , and the constant

<span id="page-26-1"></span>
$$
C_{n,V,H} := (1 + ||V||)^2 ||\widetilde{V}||_n^{n-1}.
$$

If supp  $f \subseteq [-a, a]$ , then the fundamental theorem of calculus gives

$$
|| (fu^p)^{(p)}||_{\infty} \le 2a || (fu^p)^{(p+1)}||_{\infty}.
$$

Since  $(fu^{p+1})(p+1) = (fu^p)(p+1)u + (p+1)(fu^p)(p)$ , we obtain

$$
||(fu^{p+1})^{(p+1)}||_{\infty} \le (|u(a)| + 2a(p+1))||(fu^p)^{(p+1)}||_{\infty}.
$$

Along with [\(68\)](#page-26-1), the latter two inequalities yield the result for  $n \geq 3$ .

If  $n = 1$ , then  $p = 0$  and [\(55\)](#page-21-4) gives  $\tilde{R}_{1,H,f}^0(V_k) - \tilde{R}_{1,H,f}^0(W) = f(H + V_k)$  $f(H+W)$ . Hence, by Theorem [3.12](#page-14-0) and the fundamental theorem of calculus,

$$
\widetilde{R}_{1,H,f}^{0}(V_{k}) - \widetilde{R}_{1,H,f}^{0}(W) = \int_{0}^{1} T_{f^{[1]}}^{H_{t},H_{t}}(V_{k} - W) dt,
$$

where  $H_t = H + W + t(V_k - W)$ . By [\(22\)](#page-12-3) of Theorem [3.10](#page-12-0) [\(i\)](#page-12-1) for  $j = 1$  applied to  $T_{f[1]}^{H_t, H_t}(V_k - W)$  and by continuity of the trace, we obtain

$$
\operatorname{Tr}(\widetilde{R}_{1,H,f}^{0}(V_{k}) - \widetilde{R}_{1,H,f}^{0}(W)) = \int_{0}^{1} \left( \operatorname{Tr}(T_{(fu)}^{H_{t},H_{t}}((V_{k}-W)(H_{t}-iI)^{-1})) - \operatorname{Tr}(f(H_{t})(V_{k}-W)(H_{t}-iI)^{-1}) \right) dt.
$$

Noticing that

$$
\sup_{t \in [0,1]} \|(V_k - W)(H_t - iI)^{-1}\|_1 \le (1 + \|V_k - W\|) \|\widetilde{V}_k - \widetilde{W}\|_1
$$
  

$$
\le (1 + 2\|V\|) \|\widetilde{V}_k - \widetilde{W}\|_1
$$

and applying Hölder's inequality and the Riesz–Markov representation theorem completes the proof of the result for  $n = 1$ .

Below we extend the result of Proposition [4.6](#page-22-2) to relative Schatten class perturbations.

*Proof of Proposition* [4.4](#page-21-2). Let  $(V_k)_k$  be a sequence provided by Lemma [4.8.](#page-23-0) For every  $p \in \{0, \ldots, n-1\}$  and  $k \in \mathbb{N}$ , let  $\breve{\eta}_{p,k}$  be a function satisfying

$$
\operatorname{Tr}(\widetilde{R}_{n,H,f}^p(V_k)) = \int (fu^p)^{(p+1)}(x)\check{\eta}_{p,k}(x)\,dx,
$$

which exists by Proposition [4.6.](#page-22-2) By Lemma [4.9](#page-24-0) applied to  $W = V_m$ , we have

$$
\|\check{\eta}_{p,k} - \check{\eta}_{p,m}\|_{L^1((-a,a))} = \sup_{\substack{f \in C_c^{n+1}[-a,a] \\ \| (fu^p)^{(p+1)} \|_{\infty} \le 1}} |\operatorname{Tr}(\widetilde{R}_{n,H,f}^p(V_k) - \widetilde{R}_{n,H,f}^p(V_m))|
$$
  

$$
\le c_{n,H,V,a} \|\widetilde{V}_k - \widetilde{V}_m\|_n.
$$

By Lemma [4.8,](#page-23-0) the latter expression approaches 0 as  $k \ge m \to \infty$ . Thus,  $(\check{\eta}_{p,k})_k$  is Cauchy in  $L^1_{loc}(\mathbb{R})$ . Let  $\breve{\eta}_p$  be its  $L^1_{loc}$ -limit.

Assume that  $f \in C_c^{n+1}[-a, a]$ . We obtain

$$
\int_{\mathbb{R}} \tilde{\eta}_p(x) (fu^p)^{(p+1)}(x) dx = \int_{\text{supp } f} (fu^p)^{(p+1)}(x) \tilde{\eta}_p(x) dx
$$
\n
$$
= \lim_{k \to \infty} \int_{\text{supp } f} (fu^p)^{(p+1)}(x) \tilde{\eta}_{p,k}(x) dx
$$
\n
$$
= \lim_{k \to \infty} \text{Tr}(\tilde{R}_{n,H,f}^p(V_k)).
$$

 $\blacksquare$ 

By Lemma [4.9](#page-24-0) applied to  $W = V$ ,

$$
|\operatorname{Tr}(\widetilde{R}_{n,H,f}^p(V_k) - \widetilde{R}_{n,H,f}^p(V))| \le c_{n,H,V,a} \|(fu^p)^{(p+1)}\|_{\infty} \|\widetilde{V}_k - \widetilde{V}\|_{n}
$$

for every  $k \in \mathbb{N}$ . Hence, by Lemma [4.8,](#page-23-0)

$$
\operatorname{Tr}(\widetilde{R}_{n,H,f}^p(V)) = \lim_{k \to \infty} \operatorname{Tr}(\widetilde{R}_{n,H,f}^p(V_k)) = \int_{\mathbb{R}} (fu^p)^{(p+1)}(x)\check{\eta}_p(x) dx,
$$

completing the proof of the result.

## 4.3. Absolute continuity of the spectral shift measure

In this section we prove our main result for relative Schatten class perturbations.

*Proof of Theorem* [4.1](#page-15-0). Let  $f \in C_c^{n+1}$ . We provide a proof in the case  $n \geq 3$ ; the cases  $n = 1$  and  $n = 2$  can be proved completely analogously. Applying the general Leibniz differentiation rule on the right-hand side of  $(54)$  (see Proposition [4.4\)](#page-21-2) gives

$$
\begin{split} &\text{Tr}(R_{n,H,f}(V))\\ &= \sum_{p=0}^{n-1} (-1)^{n-1-p} \int_{\mathbb{R}} (fu^p)^{(p+1)}(x) \check{\eta}_p(x) \, dx. \\ &= \sum_{p=0}^{n-1} (-1)^{n-1-p} \sum_{k=0}^{p+1} \int_{\mathbb{R}} \binom{p+1}{k} f^{(k)}(x) (u^p)^{(p+1-k)}(x) \check{\eta}_p(x) \, dx \\ &= \sum_{p=0}^{n-1} (-1)^{n-1-p} \sum_{k=1}^{p+1} \int_{\mathbb{R}} f^{(k)}(x) \binom{p+1}{k} \frac{p!}{(k-1)!} u^{k-1}(x) \check{\eta}_p(x) \, dx. \end{split}
$$

Integration by parts gives

$$
\text{Tr}(R_{n,H,f}(V)) = \sum_{p=0}^{n-1} \int_{\mathbb{R}} f^{(p+1)}(x) \tilde{\eta}_p(x) \, dx,
$$

where

$$
\widetilde{\eta}_p(t) = \sum_{k=0}^{p+1} \frac{(-1)^{n-k} p! (p+1)!}{(p+1-k)! k! (k-1)!} \int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{p-k}} u^{k-1}(x) \widetilde{\eta}_p(x) dx.
$$

Subsequent integration by parts gives

$$
\text{Tr}(R_{n,H,f}(V))
$$
\n
$$
= \int_{\mathbb{R}} f^{(n)}(x) \left( \sum_{p=0}^{n-1} (-1)^{n-1-p} \int_{0}^{x} ds_1 \int_{0}^{s_1} ds_2 \cdots \int_{0}^{s_{n-p-2}} \tilde{\eta}_p(t) dt \right) dx
$$
\n
$$
=: \int_{\mathbb{R}} f^{(n)}(x) \tilde{\eta}_n(x) dx \tag{69}
$$

for every  $f \in C_c^{n+1}$ . Since  $\eta_p \in L^1_{loc}$  (see Proposition [4.4\)](#page-21-2), we have that  $\tilde{\eta}_p \in L^1_{loc}$ and, hence,  $\dot{\eta}_n \in L^1_{loc}$ .

By Proposition [4.2,](#page-16-0) there exists a locally finite Borel measure  $\mu_n$  satisfying [\(35\)](#page-16-2) and determined by [\(35\)](#page-16-2) for every  $f \in C_c^{n+1}$  uniquely up to an absolutely continuous measure whose density is a polynomial of degree at most  $n - 1$ . Combining the latter with [\(69\)](#page-29-0) implies

<span id="page-29-0"></span>
$$
d\mu_n(x) = \dot{\eta}_n(x)dx + p_{n-1}(x)dx =: \dot{\eta}_n(x)dx,\tag{70}
$$

where  $p_{n-1}$  is a polynomial of degree at most  $n - 1$ . By Proposition [4.2,](#page-16-0) the function  $m_n := \hat{\eta}_n + p_{n-1}$  satisfies [\(34\)](#page-16-1) for every  $f \in \mathfrak{W}_n$ . The fact that  $u^{-n-\varepsilon} d\mu_n$  is a finite measure translates to  $\acute{\eta}_n \in L^1(\mathbb{R}, u^{-n-\epsilon}(x)dx)$ .

It follows from [\(36\)](#page-16-4) that

$$
||u^{-n-\varepsilon} d\mu_n|| \leq ||u^{-\varepsilon}||_{\infty} ||\nu_n|| + ||u^{-n-\varepsilon}\xi_n||_1.
$$

Along with [\(37\)](#page-17-2) and [\(38\)](#page-17-1), the latter implies

$$
||u^{-n-\varepsilon} d\mu_n|| \leq c_n (1+||u^{-1-\varepsilon}||_1)(1+||V||) ||V(H-iI)^{-1}||_n^n.
$$

Since

$$
\int_{0}^{1} (1+x^2)^{(-1-\varepsilon)/2} dx \le 1 \quad \text{and} \quad \int_{1}^{\infty} (1+x^2)^{(-1-\varepsilon)/2} dx \le \int_{1}^{\infty} x^{-1-\varepsilon} dx = \varepsilon^{-1},\tag{71}
$$

we obtain the bound

$$
||u^{-n-\varepsilon} d\mu_n|| \leq c_n (1+\varepsilon^{-1})(1+||V||) ||V(H-iI)^{-1}||_n^n,
$$
 (72)

which translates to

$$
\int_{\mathbb{R}} |\dot{\eta}_n(x)| \frac{dx}{(1+|x|)^{n+\varepsilon}} \leq c_n (1+\varepsilon^{-1})(1+\|V\|) \|V(H-iI)^{-1}\|_n^n.
$$

We define

<span id="page-30-2"></span>
$$
\eta_n := \text{Re}(\eta_n),
$$

and obtain [\(33\)](#page-15-4) by using  $|\eta_n| \leq |\eta_n|$ . As we have seen,  $\eta_n$  satisfies [\(34\)](#page-16-1) for all  $f \in \mathfrak{W}_n$ . Therefore,

$$
\text{Tr}(R_{n,H,f}(V)) = \int_{\mathbb{R}} f^{(n)}(x)\eta_n(x) \, dx + i \int_{\mathbb{R}} f^{(n)}(x) \, \text{Im}(\eta_n(x)) \, dx. \tag{73}
$$

When  $f \in \mathfrak{W}_n$  is real-valued, the left-hand side of [\(73\)](#page-30-2) is real, and consequently the second term on the right-hand side of [\(73\)](#page-30-2) vanishes. The latter implies [\(34\)](#page-16-1) for realvalued  $f \in \mathfrak{W}_n$ . By applying [\(34\)](#page-16-1) to the real-valued functions Re(f) and Im(f), we extend [\(34\)](#page-16-1) to all  $f \in \mathfrak{W}_n$ .

The uniqueness of  $\eta_n$  satisfying [\(34\)](#page-16-1) up to a polynomial summand of order at most  $n - 1$  can be established completely analogously to the uniqueness of the measure  $\mu_n$ established in Proposition [4.2.](#page-16-0)

## <span id="page-30-1"></span>5. Examples

We discuss models of noncommutative geometry and mathematical physics that satisfy the condition [\(1\)](#page-1-0).

## <span id="page-30-0"></span>5.1. Noncommutative geometry

In this section we show that the relative Schatten class condition occurs naturally in noncommutative geometry, namely, in inner perturbations of regular locally compact spectral triples (see Definition [5.1](#page-30-3) below). Many examples, including noncommutative field theory [\[6\]](#page-34-17), satisfy the following definition.

Let dom $(D)$  denote the domain of any operator D and let

$$
\delta_D(T) := [|D|, T]
$$

be defined on those  $T \in \mathcal{B}(\mathcal{H})$  for which  $\delta_D(T)$  extends to a bounded operator.

<span id="page-30-3"></span>**Definition 5.1.** A *locally compact spectral triple*  $(A, H, D)$  consists of a separable Hilbert space  $\mathcal{H}$ , a self-adjoint operator D in  $\mathcal{H}$  and a \*-algebra  $\mathcal{A} \subseteq B(\mathcal{H})$  such that  $a(\text{dom}(D)) \subseteq \text{dom}(D), [D, a]$  extends to a bounded operator, and  $a(D - iI)^{-s} \in S^1$ for all  $a \in \mathcal{A}$  and some  $s \in \mathbb{N}$ , called the *summability* of  $(\mathcal{A}, \mathcal{H}, D)$ . A spectral triple  $(A, \mathcal{H}, D)$  is called *regular* if for all  $a \in A$ , we have  $a, [D, a] \in \bigcap_{k=1}^{\infty} \text{dom}(\delta_D^k)$ .

The following result appears to be known, but nowhere explicitly proven, although a similar statement is made in [\[23\]](#page-35-6).

Let  $\Omega_D^1(\mathcal{A}) := \{ \sum_{j=1}^n a_j [D, b_j] : a_j, b_j \in \mathcal{A}, n \in \mathbb{N} \}$  denote the set of inner fluctuations [\[2\]](#page-34-6) or *Connes' differential one-forms*.

**Theorem 5.2.** A regular locally compact spectral triple  $(A, \mathcal{H}, D)$  of summability s *satisfies*  $V(D - iI)^{-1} \in S^s$  for all  $V \in \Omega_D^1(\mathcal{A})$ .

*Proof.* Let  $V = \sum_{j=1}^{n} a_j [D, b_j] \in \Omega_D^1(\mathcal{A})$  be arbitrary and let  $\delta := \delta_D$ . For all  $X \in \Omega$  $\bigcap_{k=1}^{\infty}$  dom $(\delta^k)$  we have

$$
X(|D|-iI)^{-1} = (|D|-iI)^{-1}X + (|D|-iI)^{-1}\delta(X)(|D|-iI)^{-1}.
$$

By induction, for all  $X \in \bigcap_{k=1}^{\infty} \text{dom}(\delta^k)$  there exists some  $Y \in \bigcap_{k=1}^{\infty} \text{dom}(\delta^k)$  such that

$$
X(|D|-iI)^{-s} = (|D|-iI)^{-s}Y.
$$
\n(74)

<span id="page-31-0"></span>:

Since  $[D, b_j] \in \bigcap_{k=1}^{\infty} \text{dom}(\delta^k)$  for all j and since  $g: \mathbb{R} \to \mathbb{C}$ ,  $t \mapsto (|t| - i)/(t - i)$ is continuous and bounded, we have  $g(D) \in \mathcal{B}(\mathcal{H})$  and there exists some  $Y_j \in \mathcal{B}(\mathcal{H})$ such that

$$
V(D - iI)^{-s} = \sum_{j} a_j [D, b_j] (|D| - iI)^{-s} g(D)^s
$$
  
= 
$$
\sum_{j} a_j (|D| - iI)^{-s} Y_j g(D)^s
$$
  
= 
$$
\sum_{j} a_j (D - iI)^{-s} g(D)^{-s} Y_j g(D)^s \in S^1
$$

More generally, let  $X_1, \ldots, X_m \in \bigcap_{k=1}^{\infty} \text{dom}(\delta^k)$ , let  $k_1, \ldots, k_m \in \mathbb{N}$  and set  $k = \sum_{j=1}^{m} k_j$ . By induction, noting that  $\bigcap_{k=1}^{\infty}$  dom $(\delta^k)$  is an algebra, and applying [\(74\)](#page-31-0) to  $s = k_i$ , we obtain

$$
\prod_{j=1}^{m} X_j (D - iI)^{-k_j} = (D - iI)^{-k} Y,
$$

for some  $Y \in \bigcap_{k=1}^{\infty} \text{dom}(\delta^k)$ . If s is even, we obtain

$$
|(D+iI)^{-1}V^*|^s = V(D^2+I)^{-1}V^* \dots V(D^2+I)^{-1}V^*
$$
  
=  $V(D-iI)^{-s}Y \in S^1$ ,

for some  $Y \in \bigcap_{k=1}^{\infty} \text{dom}(\delta^k)$ . Therefore,

$$
V(D - iI)^{-1} = ((D + iI)^{-1}V^*)^* \in \mathcal{S}^s.
$$

П

If s is odd, we use polar decomposition to obtain  $U \in \mathcal{B}(\mathcal{H})$  such that

$$
|V(D - iI)^{-1}| = UV(D - iI)^{-1}.
$$

Hence,

$$
|V(D - iI)^{-1}|^{s} = UV(D - iI)^{-1}|V(D - iI)^{-1}|^{s-1}
$$
  
=  $UV(D^{2} + I)^{-1}V^{*} \dots V(D^{2} + I)^{-1}V^{*}V(D - iI)^{-1}$   
=  $UV(D - iI)^{-s}Y' \in \mathcal{S}^{1}$ 

for some  $Y' \in \bigcap_{k=1}^{\infty} \text{dom}(\delta^k)$ . Therefore,  $V(D - iI)^{-1} \in \mathcal{S}^s$ .

# <span id="page-32-0"></span>5.2. Differential operators

In this section we consider conditions sufficient for perturbations of Dirac and Schrödinger operators to satisfy [\(1\)](#page-1-0).

Given  $v \in L^{\infty}(\mathbb{R}^d)$ , let  $M_v$  denote the operator of multiplication by v, that is,

$$
M_v(g) := vg, \quad g \in L^2(\mathbb{R}).
$$

We will consider self-adjoint perturbations  $V = M_v$ , where v is real-valued.

Let

$$
\Delta = \sum_{k=1}^{d} \frac{\partial^2}{\partial x_k^2}
$$

denote the Laplacian operator densely defined in the Hilbert space  $L^2(\mathbb{R}^d)$ .

For  $m \geq 0$ , let  $D_m$  denote the free massive Dirac operator defined as follows. For  $d \in \mathbb{N}$ , let  $N(d) := 2^{\lfloor (d+1)/2 \rfloor}$ . Let  $e_k \in M_{N(d)}(\mathbb{C})$ ,  $0 \le k \le d$ , be the Clifford generators, that is, self-adjoint matrices satisfying  $e_k^2 = I$  for  $0 \le k \le d$  and  $e_{k_1}e_{k_2} =$  $-e_{k_2}e_{k_1}$  for  $0 \le k_1, k_2 \le d$ , such that  $k_1 \ne k_2$ . Let  $D_k := \frac{\partial}{i \partial x_k}$ . Then, the operator

$$
D_m := e_0 \otimes mI + \sum_{k=1}^d e_k \otimes D_k
$$

is densely defined in the Hilbert space  $\mathbb{C}^{N(d)} \otimes L^2(\mathbb{R}^d)$ .

We note that  $D_0$  is unitarily equivalent to  $I \otimes D$ , where  $I \in M_{N(d)/N(d-1)}(\mathbb{C})$ and D is the usual massless Dirac operator. We also note that, in the case when  $d = 1$ , the Dirac operator  $D_0 = I \otimes \frac{\partial}{\partial x}$  can be identified with the differential operator  $\frac{\partial}{\partial x}$ in the Hilbert space  $L^2(\mathbb{R})$ .

The Schatten class membership of the weighted resolvents below was derived in [\[20,](#page-35-7) Theorem 3.3 and Remark 3.6]. To estimate the respective Schatten norms one just needs to carefully follow the proof of the latter result.

<span id="page-33-2"></span>**Theorem 5.3.** Let  $d \in \mathbb{N}$ ,  $1 \leq p < \infty$ . Let

$$
v \in \begin{cases} \ell^p(L^2(\mathbb{R}^d)) \cap L^\infty(\mathbb{R}^d) & \text{if } 1 \le p < 2 \\ L^p(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d) & \text{if } 2 \le p < \infty \end{cases}
$$

*be real-valued.*

i. If 
$$
p > d
$$
 and  $m \ge 0$ , then  $(I \otimes M_v)(D_m - iI)^{-1} \in S^p$  and

$$
||(I \otimes M_v)(D_m - iI)^{-1}||_p \le c_{d,p} \begin{cases} ||v||_{\ell^p(L^2)} & \text{if } 1 \le p < 2, \\ ||v||_{L^p} & \text{if } 2 \le p < \infty. \end{cases} (75)
$$

ii. If 
$$
p > \frac{d}{2}
$$
, then  $M_v(-\Delta - iI)^{-1} \in \mathcal{S}^p$  and

<span id="page-33-1"></span><span id="page-33-0"></span>
$$
||M_v(-\Delta - iI)^{-1}||_p \le c_{d,p} \begin{cases} ||v||_{\ell^p(L^2)} & \text{if } 1 \le p < 2, \\ ||v||_{L^p} & \text{if } 2 \le p < \infty. \end{cases} \tag{76}
$$

Remark 5.4. The bounds analogous to [\(75\)](#page-33-0) and [\(76\)](#page-33-1) can also be established for perturbed Dirac  $D_m + W$  and perturbed Schrödinger  $-\Delta + W$  operators, respectively. The respective results follow from Theorem [5.3](#page-33-2) and Proposition [5.5](#page-33-3) below. In particular, we have the following bound for a massive Dirac operator with electromagnetic potential in the case  $p > d$ :

$$
\left\| (I \otimes M_v) \left( D_m + \sum_{k=1}^d e_k \otimes M_{w_k} + I \otimes M_{w_{d+1}} - iI \right)^{-1} \right\|_p
$$
  
\$\leq c\_{d,p}(1 + \max\_{1 \leq k \leq d+1} \|w\_k\|\_{L^{\infty}}) \begin{cases} \|v\|\_{\ell^p(L^2)} & \text{if } 1 \leq p < 2, \\ \|v\|\_{L^p} & \text{if } 2 \leq p < \infty. \end{cases}

The same reasoning applies to generalized Dirac operators  $I_k \otimes D + W$ , where  $k \in \mathbb{N}$ and  $W \in \mathcal{B}(\mathbb{C}^k \otimes \mathcal{H})_{sa}$ , that are associated with almost-commutative spectral triples.

<span id="page-33-3"></span>**Proposition 5.5.** Let H, V be self-adjoint operators in H and  $W \in \mathcal{B}(\mathcal{H})_{sa}$ . Let  $1 \leq p < \infty$  and assume that  $||V(H - iI)^{-1}||_p < \infty$ . Then,

$$
||V(H + W - iI)^{-1}||_p \le ||V(H - iI)^{-1}||_p(1 + ||W||).
$$

*Proof.* The result follows from the second resolvent identity

$$
(H + W - iI)^{-1} = (H - iI)^{-1} - (H - iI)^{-1}W(H + W - iI)^{-1}
$$

upon multiplying it by  $V$  and applying Hölder's inequality for Schatten norms.

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