

## Divided differences in noncommutative geometry: Rearrangement Lemma, functional calculus and expansional formula

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**Abstract.** We state a generalization of the Connes–Tretkoff–Moscovici Rearrangement Lemma and give a surprisingly simple (almost trivial) proof of it. Secondly, we put on a firm ground the multivariable functional calculus used implicitly in the Rearrangement Lemma and elsewhere in the recent modular curvature paper by Connes and Moscovici [3]. Furthermore, we show that the fantastic formulas connecting the one and two variable modular functions of loc. cit. are just examples of the plenty recursion formulas which can be derived from the calculus of divided differences. We show that the functions derived from the main integral occurring in the Rearrangement Lemma can be expressed in terms of divided differences of the Logarithm, generalizing the “modified Logarithm” of Connes–Tretkoff [4].

Finally, we show that several expansion formulas related to the Magnus expansion [13] have a conceptual explanation in terms of a multivariable functional calculus applied to divided differences.

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### 1. Introduction

This paper is inspired by the recent work on the spectral geometry of non-commutative tori [3, 4, 7, 8].

The striking novelty of the paper [3] is the occurrence of universal one and two variable functions  $K_0(s)$ ,  $H_0(s, t)$  in the expression for the second heat coefficient [3, (1)]<sup>1</sup>

$$a_2(a, \Delta_\varphi) = \text{Const} \cdot \varphi_0 \left( a \left( K_0(\nabla)(\Delta h) + \frac{1}{2} H_0(\nabla_1, \nabla_2)(\square_{\mathfrak{R}}(h)) \right) \right). \quad (1.1)$$

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A rather fantastic aspect is that these functions satisfy relations of the kind [3, (4)]<sup>2</sup>

$$H(a, b) = \frac{K(b) - K(a)}{a + b} + \frac{K(a + b) - K(b)}{a} - \frac{K(a + b) - K(a)}{b}. \quad (1.2)$$

Eq. (1.2) is proved in loc. cit. by an a priori argument [3, Sec. 4.3].

On the other hand Eq. (1.2) is a sum of *divided differences*. Namely, noting that  $K$  in loc. cit. is an even function, we can rewrite Eq. (1.2) as

$$H(a, b) = [-a, b]K + [a + b, b]K - [a + b, a]K. \quad (1.3)$$

So it seems as if divided differences could be the key to a lot of the somewhat magic formulas occurring in this business. And indeed when thinking about [3] for a while the author noticed that one stumbles over divided differences everywhere, notably in the noncommutative Taylor expansion formula of the exponential function and in concrete functions related to the Rearrangement Lemma, and soon it became obvious that the role of divided differences in the subject needs to be clarified.

Divided differences are a standard tool in numerical analysis and they can be calculated quite efficiently. We will recall the main facts about them in Appendix A below. To the best of our knowledge their appearance in operator theory and functional calculus is new. In a different context, however, it was also observed in [1] that the Magnus expansion formula can be interpreted in terms of the Genocchi–Hermite formula and hence related to divided differences.

We now describe the content of the paper in more detail.

**1.1. Rearrangement Lemma and multivariable functional calculus.** An important technical tool for the calculation of heat coefficients in the noncommutative setting is the Rearrangement Lemma which informally reads

$$\begin{aligned} & \int_0^\infty f_0(uk^2) \cdot b_1 \cdot f_1(uk^2) \cdot b_2 \cdot \dots \cdot b_p \cdot f_p(uk^2) du \\ &= k^{-2} F(\Delta^{(1)}, \Delta^{(1)} \Delta^{(2)}, \dots, \Delta^{(1)} \cdot \dots \cdot \Delta^{(p)})(b_1 \cdot \dots \cdot b_p), \end{aligned} \quad (1.4)$$

where the function  $F(s_1, \dots, s_p)$  is

$$F(s) = \int_0^\infty f_0(u) \cdot f_1(us_1) \cdot \dots \cdot f_p(us_p) du$$

and  $\Delta^{(j)}$  signifies that the modular operator  $\Delta = k^{-2} \cdot k^2$  acts on the  $j$ -th factor.

<sup>1</sup> $\varphi_0$  is the natural trace on the non-commutative torus,  $\Delta$  is the flat Laplacian,  $\Delta_\varphi$  the conformal Laplacian with respect to the non-tracial weight  $\varphi(a) = \varphi_0(ae^{-h})$ ,  $\Delta = e^{-h} \cdot e^h$  denotes the modular operator,  $\nabla = \log \Delta$ .  $\square_{\mathbb{R}}(h)$  is the Dirichlet quadratic form in  $\delta_1 h, \delta_2 h$ , where  $\delta_1, \delta_2$  are the natural derivations associated to the  $\mathbb{R}^2$ -action on the non-commutative torus. Finally,  $\nabla_j$  signifies that  $\nabla_j$  acts on the  $j$ -th factor.  $e^h =: k^2$ .

<sup>2</sup> $H$  and  $K$  are modifications of  $H_0$  and  $K_0$ , for details see loc. cit.

In [3] it is proved for the concrete integral

$$\int_0^\infty (uk^2)^{|\alpha|+p-1} (1+uk^2)^{-\alpha_0-1} \cdot b_1 \cdot (1+uk^2)^{-\alpha_1-1} \cdot \dots \cdot b_p \cdot (1+uk^2)^{-\alpha_p-1} du, \tag{1.5}$$

and the function

$$H_\alpha^{(p)}(s, m) := \int_0^\infty x^{|\alpha|+p-1-m} \cdot (1+x)^{-\alpha_0-1} \cdot \prod_{j=1}^p (1+s_j x)^{-\alpha_j-1} dx. \tag{1.6}$$

The Rearrangement Lemma and the function  $H_\alpha^{(p)}(s, m)$  are crucial for identifying the ingredients of Eq. (1.1) from a combinatorially challenging expression for the resolvent expansion. The one and two variable functions mentioned above are, after a change of variables, simple linear combinations of basic  $H_\alpha^{(p)}(s, m)$  for a few values of  $\alpha$ .

The proof of Eq. (1.6) in loc. cit. consists of an intimidating calculation involving explicit Fourier transforms of the factors of the integrand after a change of variables. Since the Lemma has appeared in several versions of increasing complexity in the literature, [4, Lemma 6.2], [3, Lemma 6.2], [7, Lemma 4.2], [2, Prop. 3.4], [8, Lemma 4.1], we think that a systematic treatment might be in order, also in light of possible generalizations of the aforementioned papers to other noncommutative spaces.

One of the purposes of this note is to give a new proof of a fairly general version of this Lemma. Our proof is not at all shorter than the one in [3, Lemma 6.2] but, at least the author believes so, conceptually much simpler. We do not need explicit Fourier transforms, all we use is the Spectral Theorem and the trivial substitution  $\int_0^\infty f(u\lambda) du = \lambda^{-1} \int_0^\infty f(u) du$ . Namely, the Rearrangement Lemma is concerned with an integral,

$$\int_0^\infty f(uR_0, uR_1, \dots, uR_n) du, \tag{1.7}$$

where  $R_0, \dots, R_n$  are commuting selfadjoint operators, and it ultimately boils down to the justification of the “operator substitution”  $\tilde{u} = uR_0, du = R_0^{-1} d\tilde{u}$ .

Secondly, we would like to put on a firm ground the functional calculus which is implicitly used by the statement “ $\Delta^{(j)}$  signifies that  $\Delta$  acts on the  $j$ -th factor”. The authors hopes that the current modest considerations will serve the community as he has even heard the statement “that these formulas should be considered as formal since they are not based on a valid functional calculus”. We will see that one should not be that pessimistic and that the proper way to make sense of the notation  $F(\Delta^{(1)}, \dots)$  is the theory of tensor products of Banach and  $C^*$ -algebras and the functional calculus for several commuting operators. At the heart of the problem is the multiplication map

$$\mu_n : \mathcal{A}^{\otimes n+1} \ni a_0 \otimes \dots \otimes a_n \mapsto a_0 \cdot \dots \cdot a_n \tag{1.8}$$

and the problem of extending it in a proper way to tensor product completions. More concretely,  $\mu_n$  extends by continuity to the projective Banach algebra tensor product  $\mathcal{A}_\gamma^{\otimes n+1}$ . On the other hand a nice functional calculus for commuting selfadjoint operators is available in the maximal  $C^*$ -tensor product  $\mathcal{A}_\pi^{\otimes n+1}$ . We suspect, however, that  $\mu_n$  does not extend by continuity to  $\mathcal{A}_\pi^{\otimes n+1}$ . We circumvent this problem by establishing, for a selfadjoint element  $a \in \mathcal{A}$ , a smooth functional calculus in  $\mathcal{A}_\gamma^{\otimes n+1}$  for the commuting elements  $a^{(j)} = 1_{\mathcal{A}} \otimes \cdots \otimes a \otimes \cdots$  ( $a$  in slot  $j$  counted from 0).

**1.2. Divided differences.** Coming back to divided differences and the formulas Eq. (1.2) and (1.3) we will show below that when dealing with the integrand of Eq. (1.6), divided difference occur in abundance and the calculus of divided differences leads to a more or less endless list of variations of Eq. (1.3).

More concretely, we will express the function Eq. (1.6) explicitly in terms of divided differences of the Logarithm:

$$H_\alpha^{(p)}(s, m) = (-1)^{m+|\alpha|+p-1} \cdot [1^{\alpha_0+1}, s_1^{\alpha_1+1}, \dots, s_p^{\alpha_p+1}] \text{id}^m \log. \quad (1.9)$$

The modified logarithm  $\mathcal{L}_m$  of [4, Lemma 3.2] is nothing but the divided difference

$$\mathcal{L}_m(s) = (-1)^m \cdot [1^{m+1}, s] \log = (-1)^m \cdot [1^m, s] \mathcal{L}_0, \quad \mathcal{L}_0(s) = \frac{\log(s)}{s-1}, \quad (1.10)$$

where  $[1^m, s]f$  is an abbreviation for the divided difference  $[1, \dots, 1, s]f$  with  $m$  repetitions of 1, cf. Secs. 5.1.2 and A.2. Note that  $\mathcal{L}_0(e^x)$  is the generating function for the Bernoulli numbers, which occurs prominently in [3]<sup>3</sup>.

**1.3. Noncommutative Taylor expansion of the exponential function.** We show that the expansion formula for noncommutative variables  $a$  and  $b$  (cf., e.g. [3, Sec. 6.1])

$$e^{a+b} = e^a + \sum_{n=1}^{\infty} \int_{0 \leq s_n \leq \dots \leq s_1 \leq 1} e^{(1-s_1)a} \cdot b \cdot e^{(s_1-s_2)a} \cdot b \cdot \dots \cdot b \cdot e^{s_n a} ds \quad (1.11)$$

can be interpreted nicely as an operator valued version of Newton's interpolation formula involving divided differences

$$e^{a+b} = \sum_{n=0}^{\infty} ([a^{(0)}, \dots, a^{(n)}] \exp_\gamma)(b \cdot \dots \cdot b). \quad (1.12)$$

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<sup>3</sup>To be precise with  $f(x) = \mathcal{L}_0(e^x)$  we have

$$\frac{1}{8} K(s) = \sum_{n=1}^{\infty} \frac{B_{2n}}{(2n)!} s^{2n-2} = \frac{1}{s} (f(s) - f(0) - f'(0)s) = [0, s]f - [0, 0]f = s[0, 0, s]f.$$

This immediately leads to the following generalization

$$f(a + b) \sim_{b \rightarrow 0} \sum_{n=0}^{\infty} ([a^{(0)}, \dots, a^{(n)}] f_\gamma)(b \cdot \dots \cdot b), \quad (1.13)$$

for selfadjoint elements in a  $C^*$ -algebra and a Schwartz function  $f$ . The linear term in this expansion formula is at the heart of the relations Eq. (1.2), (1.3). As an application we give a conceptually new proof of the corresponding results in [3, Lemma 4.11 and Lemma 4.12].

**1.4. Explicit examples.** Finally, in Sec. 5 we discuss explicit examples of one and two variable functions derived from Eq. (1.3) and compare them to the explicit formulas given at the end of [3]. In the preparation of Sec. 5 we used the open source computer algebra system Maxima. However, the results as they stand can be checked (a posteriori) by hand.

**1.5.** This paper is a byproduct of a recent joint project with Henri Moscovici [12]; it is used in some of the concrete calculations in Sec. 4 of that paper.

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## 2. An abstract operator substitution lemma

**2.1. Notation.**  $\mathbb{N} = \{0, 1, 2, \dots\}$ ,  $\mathbb{Z}$ ,  $\mathbb{R}$ ,  $\mathbb{C}$  denotes the natural numbers, integers, real and complex numbers resp.  $\mathbb{R}_{\geq 0}$  denotes  $\{x \in \mathbb{R} \mid x \geq 0\}$ ,  $\mathbb{R}_{> 0}$ ,  $\mathbb{R}_{< 0}$ ,  $\mathbb{Z}_{> 0}$ ,  $\mathbb{Z}_{\geq 0}$  etc. is used accordingly. Instead of the clumsy  $(\mathbb{R}_{\geq 0})^n$  we write  $\mathbb{R}_{\geq 0}^n$ .

We will frequently use the multiindex notation for partial derivatives and factorials. Recall that if  $\alpha = (\alpha_0, \dots, \alpha_n) \in \mathbb{N}^{n+1}$  is a multiindex then one abbreviates  $\alpha! := \prod_j \alpha_j!$ ,  $|\alpha| := \sum \alpha_j$ , and  $\partial_x^\alpha = \prod_j \partial_{x_j}^{\alpha_j}$ ,  $x = (x_0, \dots, x_n)$ . Furthermore, we use the Pochhammer symbol for the rising and falling factorial powers, see Eq. (B.1), (B.2).

**2.2.** Let  $\mathcal{H}$  be a Hilbert space and let  $R_0, \dots, R_n$ ,  $n \geq 1$ , be commuting positive selfadjoint operators in  $\mathcal{H}$ , i.e. all operators  $R_j$  are assumed to be  $\geq 0$  and invertible. These operators generate a commutative unital  $C^*$ -subalgebra,  $\mathcal{A} = C^*(I, R_0, \dots, R_n)$ , of the  $C^*$ -algebra of bounded linear operators,  $\mathcal{L}(\mathcal{H})$ , on the Hilbert space  $\mathcal{H}$ . By the Gelfand Representation Theorem, there exists a compact subset  $X \subset \prod_{j=0}^n \text{spec}(R_j) \subset \mathbb{C}^{n+1}$  and a  $*$ -isomorphism

$$\Phi : C(X) \longrightarrow C^*(I, R_0, \dots, R_n) \subset \mathcal{L}(\mathcal{H})$$

which sends the constant function 1 to the identity operator  $I$  and the function  $x \mapsto x_j$  onto the operator  $R_j$ ,  $j = 0, \dots, n$ .  $\Phi$  is called the spectral measure of  $R_0, \dots, R_n$ , cf. [16, Chap. 12]. For a continuous function  $f \in C(X)$  one writes suggestively  $f(R_0, \dots, R_n) := \Phi(f)$ .  $\Phi$  may also be viewed as an operator valued measure, cf. [16, 12.17]. We write  $dE$  for the associated resolution of the identity in the sense of loc. cit. Then  $f(R_0, \dots, R_n) = \int_X f(\lambda) dE(\lambda)$ .

For each pair of Hilbert space vectors  $x, y \in \mathcal{H}$  the spectral measure  $\Phi$  induces a complex Radon measure  $E_{x,y}$  on  $X$  by the identity

$$\langle f(R_0, \dots, R_n)x, y \rangle = \int_X f(\lambda) dE_{x,y}(\lambda), \quad f \in C(X).$$

**Lemma 2.1.** *With the previously introduced notation let  $f : \mathbb{R}_{\geq 0} \times X \rightarrow \mathbb{C}$  be a continuous function satisfying the integrability condition*

$$\int_0^\infty \sup_{\lambda \in X} |f(u, \lambda)| du < \infty. \quad (2.1)$$

Define  $F : X \rightarrow \mathbb{C}$  by the parameter integral

$$F(\lambda) := \int_0^\infty f(u, \lambda) du.$$

Then the integral  $\int_0^\infty f(u, R_0, \dots, R_n) du$  exists in the Bochner sense and equals  $F(R_0, \dots, R_n)$ .

In more suggestive notation this Lemma is a Fubini Theorem for the product measure  $dE du$ , i.e. the product of the spectral measure  $\Phi$  and the Lebesgue measure on the half line  $\mathbb{R}_{\geq 0}$ . Namely, using the integral notation with respect to the resolution of the identity it means

$$\int_0^\infty \int_X f(u, \lambda) dE(\lambda) du = \int_X \int_0^\infty f(u, \lambda) du dE(\lambda).$$

*Proof.* Let us first note that due to the integrability condition Eq. (2.1) and the Dominated Convergence Theorem the function  $F$  is indeed continuous.

To see the claimed Bochner integrability we note that  $u \mapsto f(u, R_0, \dots, R_n)$  is continuous (cf. [17, Prop. 4.10]). Furthermore, by the Spectral Theorem and the integrability condition Eq. (2.1) we have for the integral of the norm

$$\int_0^\infty \|f(u, R_0, \dots, R_n)\| du = \int_0^\infty \sup_{\lambda \in X} |f(u, \lambda)| du < \infty.$$

Thus the integral exists in the Bochner sense. Furthermore, for vectors  $x, y \in \mathcal{H}$  we have by continuity of the Bochner integral

$$\begin{aligned} \left\langle \int_0^\infty f(u, R_0, \dots, R_n) du x, y \right\rangle &= \int_0^\infty \langle f(u, R_0, \dots, R_n) x, y \rangle du \\ &= \int_0^\infty \int_X f(u, \lambda) dE_{x,y}(\lambda) du. \end{aligned} \quad (2.2)$$

The latter integral is an ordinary product integral of the Radon measure  $E_{x,y}$  and the Lebesgue measure. Again by the integrability condition Eq. (2.1) we have

$$\int_0^\infty \int_X |f(u, \lambda)| d|E_{x,y}(\lambda)| du \leq \|x\| \cdot \|y\| \cdot \int_0^\infty \sup_{\lambda \in X} |f(u, \lambda)| du < \infty,$$

hence Fubini's Theorem applies and we continue Eq. (2.2) to obtain

$$\begin{aligned} (2.2) &= \int_X \int_0^\infty f(u, \lambda) du dE_{x,y}(\lambda) \\ &= \int_X F(\lambda) dE_{x,y}(\lambda) = \langle F(R_0, \dots, R_n) x, y \rangle. \end{aligned}$$

This proves that indeed  $\int_0^\infty f(u, R_0, \dots, R_n) du = F(R_0, \dots, R_n)$ . □

**Theorem 2.2** (Operator Substitution Lemma). *Let  $R_0, \dots, R_n$  be commuting selfadjoint positive operators as in Sec. 2.2. Furthermore, let  $f : \mathbb{R}_{\geq 0}^{n+1} = (\mathbb{R}_{\geq 0})^{n+1} \rightarrow \mathbb{C}$  be a continuous function such that for each pair of positive real numbers  $0 < C_1 < C_2$  one has*

$$\int_0^\infty \sup_{\substack{C_1 \leq s_j \leq C_2 \\ 0 \leq j \leq n}} |f(us)| du < \infty. \tag{2.3}$$

Then for the functions

$$F : \mathbb{R}_{>0}^{n+1} \ni s \mapsto \int_0^\infty f(u \cdot s) du$$

and

$$G : \mathbb{R}_{>0}^n \ni \lambda \mapsto \int_0^\infty f(u, u\lambda_1, \dots, u\lambda_n) du$$

we have the identity

$$\begin{aligned} \int_0^\infty f(uR_0, uR_1, \dots, uR_n) du &= F(R_0, \dots, R_n) \\ &= R_0^{-1} G(R_0^{-1} R_1, \dots, R_0^{-1} R_n) = R_0^{-1} \int_0^\infty f(u, uR_0^{-1} R_1, \dots, uR_0^{-1} R_n) du. \end{aligned}$$

Both integrals exist in the Bochner sense.

**Remark 2.3.** We have formulated the Operator Substitution Lemma multiplicatively. There is an obvious additive analogue for integrals of the form

$$\int_{\mathbb{R}} h(x + T_0, x + T_1, \dots, x + T_n) dx = \int_{\mathbb{R}} h(x, x + T_1 - T_0, \dots, x + T_n - T_0) dx$$

for commuting selfadjoint operators  $T_0, \dots, T_n$  and appropriate functions  $f \in C_0(\mathbb{R}^{n+1})$ . We leave the details to the reader.

*Proof.* Put  $g(u, s) := f(us)$ ,  $0 < u < \infty$ ,  $s \in \mathbb{R}_{>0}^{n+1}$  and  $h(u, \lambda) := f(u, u\lambda_1, \dots, u\lambda_n)$ ,  $\lambda \in \mathbb{R}_{>0}^n$ . Then by Eq. (2.3) the Lemma 2.1 applies to both functions  $g$  and  $h$ . Furthermore,

$$\begin{aligned} F(s) &= \int_0^\infty f(us_0, us_1, \dots, us_n) du \\ &= \int_0^\infty s_0^{-1} f(u, us_0^{-1}s_1, \dots, us_0^{-1}s_n) du = s_0^{-1}G(s_0^{-1}s_1, \dots, s_0^{-1}s_n), \end{aligned}$$

and the claim follows.  $\square$

**Example 2.4.** Let  $\alpha = (\alpha_0, \dots, \alpha_p) \in \mathbb{N}^{p+1}$  be a multiindex. Then put

$$f(x_0, x_1, \dots, x_p) := x_0^\nu \cdot \prod_{j=0}^p (1 + x_j)^{-\alpha_j - 1}, \quad -1 < \nu < |\alpha| + p.$$

We show that  $f$  satisfies the integrability condition Eq. (2.3) of Theorem 2.2. Given  $0 < C_1 < C_2$  then for  $C_1 \leq s_j \leq C_2$  and  $0 \leq u \leq 1$  we have

$$|f(us)| \leq s_0^\nu \cdot u^\nu \leq \text{const} \cdot u^\nu,$$

while for  $u \geq 1$  we have

$$|f(us)| = \left| (s_0 u)^\nu \prod_{j=0}^p (s_j u)^{-\alpha_j - 1} \cdot \prod_{j=0}^p \left( \frac{s_j u}{1 + s_j u} \right)^{\alpha_j + 1} \right| \leq \text{const} \cdot |u|^{\nu - |\alpha| - p - 1},$$

hence the claim.

Inductively, one easily sees that for any multiindex  $\alpha$  the function  $\partial_s^\alpha f(us) = u^\alpha (\partial^\alpha f)(us)$  also satisfies the integrability condition Eq. (2.1).

### 3. Tensor products and the Rearrangement Lemma

#### 3.1. Projective vs. maximal $C^*$ -tensor product, the contraction map.

**3.1.1. Tensor product completions.** Let  $\mathcal{A}$  be a unital  $C^*$ -algebra. Denote by  $\mathcal{A}^{\otimes n+1} := \mathcal{A} \otimes \dots \otimes \mathcal{A}$  the  $(n+1)$ -fold algebraic tensor product. For elementary tensors we use the notations  $(a_0, \dots, a_n)$  and  $a_0 \otimes \dots \otimes a_n$  as synonyms. By

$$\mu_n : \mathcal{A}^{\otimes n+1} \rightarrow \mathcal{A}, (a_0, \dots, a_n) \mapsto a_0 \cdot \dots \cdot a_n$$

we denote the multiplication map.

We discuss the issue of extending the multiplication map to tensor product completions of  $\mathcal{A}^{\otimes n+1}$ . We denote by  $\mathcal{A}_\gamma^{\otimes n+1}$  the projective tensor product

completion of  $\mathcal{A}^{\otimes n+1}$ , cf., e.g. [9]. That is  $\mathcal{A}_\gamma^{\otimes n+1}$  is the completion of  $\mathcal{A}^{\otimes n+1}$  with respect to the norm

$$\|x\|_\gamma = \inf \sum_i \|a_0^{(i)}\| \cdot \dots \cdot \|a_n^{(i)}\|,$$

where the infimum is taken over all representations of  $x \in \mathcal{A}^{\otimes n+1}$  as a finite sum  $\sum_i (a_0^{(i)}, \dots, a_n^{(i)})$ .  $\mathcal{A}_\gamma^{\otimes n+1}$  is a Banach–algebra. Moreover, the adjoint map is easily seen to be continuous with respect to the norm  $\|\cdot\|_\gamma$ , hence  $\mathcal{A}_\gamma^{\otimes n+1}$  is a Banach–\*–algebra.

Furthermore, let  $\mathcal{A}_\pi^{\otimes n+1}$  be the maximal  $C^*$ –algebra tensor product completion of  $\mathcal{A}^{\otimes n+1}$  [17, Sec. IV.4]. That is  $\mathcal{A}_\pi^{\otimes n+1}$  is the completion of  $\mathcal{A}^{\otimes n+1}$  with respect to the norm

$$\|x\|_\pi = \sup \|\varrho(x)\|,$$

where  $\varrho$  runs through all \*–representations of  $\mathcal{A}^{\otimes n+1}$ .  $\|\cdot\|_\pi \leq \|\cdot\|_\gamma$  and hence there is a natural continuous \*–homomorphism  $\text{pr}_\pi^\gamma : \mathcal{A}_\gamma^{\otimes n+1} \rightarrow \mathcal{A}_\pi^{\otimes n+1}$  whose range is dense.

Each of the two tensor products comes with a benefit and a curse and these are mutually exclusive. The projective tensor product behaves well in the sense that  $\mu_n$  extends by continuity to a linear map  $\mathcal{A}_\gamma^{\otimes n+1} \rightarrow \mathcal{A}$ . It behaves badly in the sense that  $\mathcal{A}_\gamma^{\otimes n+1}$ , although being a Banach \*–algebra, is a  $C^*$ –algebra only in trivial cases. On the other hand the  $C^*$ –algebra  $\mathcal{A}_\pi^{\otimes n+1}$  behaves well in the sense that it is  $C^*$  and hence, e.g. there is a continuous functional calculus for commuting selfadjoint elements. It behaves badly in the sense that the author does not know whether the multiplication map  $\mu_n$  extends by continuity to  $\mathcal{A}_\pi^{\otimes n+1}$ ; in fact he suspects that there exist interesting cases where it does not extend. A poll among available experts on tensor products was inconclusive.

Needless to say, for matrix algebras the algebraic tensor product is already complete and there is no problem. Even in this seemingly trivial case the results outlined below do have aspects which, to the best of our knowledge, seem to be new.

**3.1.2. The contraction map.** We come to a crucial construction. For  $a \in \mathcal{A}_\gamma^{\otimes n+1}$  and elements  $b_1, \dots, b_n \in \mathcal{A}$  we write, motivated by [3, Lemma 6.2], cf. Eq. (1.4), suggestively

$$a(b_1 \cdot \dots \cdot b_n) := \mu_n(a \cdot (b_1 \otimes \dots \otimes b_n \otimes 1_{\mathcal{A}})) \in \mathcal{A}, \tag{3.1}$$

and call the result the contraction of  $a$  by  $b_1 \otimes \dots \otimes b_n$ .

Note that if  $a = (a_0, \dots, a_n)$  is an elementary tensor then

$$(a_0, \dots, a_n)(b_1 \cdot \dots \cdot b_n) = a_0 \cdot b_1 \cdot a_1 \cdot \dots \cdot a_{n-1} \cdot b_n \cdot a_n. \tag{3.2}$$

Eq. (3.1) induces a continuous map  $\mathcal{A}_\gamma^{\otimes n+1} \times \mathcal{A}_\gamma^{\otimes n} \rightarrow \mathcal{A}$ . The whole discussion of this section circles around the problem of extending Eq. (3.1) to a reasonable class

of elements in  $\mathcal{A}_\pi^{\otimes n+1}$ . The discussion would simplify considerably if Eq. (3.1) would extend to a continuous map  $\mathcal{A}_\pi^{\otimes n+1} \times \mathcal{A}_\pi^{\otimes n} \rightarrow \mathcal{A}$ . We do not know whether this is the case as topologies on tensor products can behave notoriously pathologic.

**3.2. Smooth functional calculus on  $\mathcal{A}_\gamma^{\otimes n+1}$ .** For  $a \in \mathcal{A}$  put  $A := e^a$  and

$$\begin{aligned} a^{(j)} &= (1_{\mathcal{A}}, \dots, 1_{\mathcal{A}}, a, 1_{\mathcal{A}}, \dots, 1_{\mathcal{A}}), & 0 \leq j \leq n \quad (a \text{ is in the } j\text{-th slot}), \\ \nabla_a^{(j)} &:= -a^{(j-1)} + a^{(j)}, & 1 \leq j \leq n, \\ \Delta_a^{(j)} &:= \exp(\nabla_a^{(j)}), & 1 \leq j \leq n, \\ &= (1_{\mathcal{A}}, \dots, 1_{\mathcal{A}}, A^{-1}, A, 1_{\mathcal{A}}, \dots, 1_{\mathcal{A}}), & (A^{-1} \text{ is in slot } j-1). \end{aligned} \tag{3.3}$$

Note that slots are enumerated starting from 0, so  $a^{(0)} = a \otimes 1_{\mathcal{A}} \otimes \dots$ ,  $a^{(1)} = 1_{\mathcal{A}} \otimes a \otimes 1_{\mathcal{A}} \otimes \dots$ , etc.

The operators  $a^{(0)}, \dots, a^{(n)}, \nabla_a^{(1)}, \dots, \nabla_a^{(n)}, \Delta_a^{(1)}, \dots, \Delta_a^{(n)}$  commute. If  $a$  is selfadjoint then so are  $a^{(j)}, \nabla_a^{(j)}, \Delta_a^{(j)}$ . Furthermore, if  $a$  is selfadjoint then  $A^{(j)} := \exp(a^{(j)})$  is positive.

The following simple identities are at the heart of the Rearrangement Lemma:

$$\begin{aligned} A^{(j)} &= (1_{\mathcal{A}}, \dots, 1_{\mathcal{A}}, A, 1_{\mathcal{A}}, \dots, 1_{\mathcal{A}}) \\ &= (AA^{-1}, \dots, AA^{-1}, A, 1_{\mathcal{A}}, \dots) \\ &= A^{(0)} \Delta^{(1)} \cdot \dots \cdot \Delta^{(j)}, & j \geq 1, \end{aligned} \tag{3.4}$$

$$a^{(j)} = a^{(0)} + \nabla_a^{(1)} + \dots + \nabla_a^{(j)}, \quad j \geq 1. \tag{3.5}$$

From now on assume that  $a \in \mathcal{A}$  is selfadjoint and let  $\Phi : C(\text{spec } a) \rightarrow \mathcal{A}$ ,  $f \mapsto f(a)$  denote the spectral measure of  $a$ . The  $(n+1)$ -fold tensor product,  $\Phi_\pi$ , is a  $*$ -isomorphism from  $C((\text{spec } a)^{n+1}) \simeq C(\text{spec } a)^{\otimes n+1}$  onto the unital  $C^*$ -subalgebra  $C^*(I, a^{(0)}, \dots, a^{(n)})$  of  $\mathcal{A}_\pi^{\otimes n+1}$  generated by  $a^{(0)}, \dots, a^{(n)}$ .  $\Phi_\pi$  is nothing but the joint spectral measure of the commuting operators  $a^{(0)}, \dots, a^{(n)}$ , e.g.  $\Phi_\pi(f) = f(a^{(0)}, \dots, a^{(n)})$ . Furthermore, this  $C^*$ -algebra also contains the operators  $\nabla_a^{(1)}, \dots, \nabla_a^{(n)}$ , and  $\Delta_a^{(1)}, \dots, \Delta_a^{(n)}$ .

If we view the operators Eq. (3.3) as elements of  $\mathcal{A}_\gamma^{\otimes n+1}$  they still admit a joint analytic functional calculus [18]. We do not make use, however, of this celebrated and somewhat demanding paper. Instead we exploit the nuclearity of Fréchet spaces of smooth functions to establish a smooth functional calculus with values in  $\mathcal{A}_\gamma^{\otimes n+1}$ . To this end let  $U \supset \text{spec } a$  be an open set. Then the algebra of smooth functions,  $C^\infty(U)$ , on  $U$  with the usual Fréchet topology is known to be nuclear [20, Sec. 51]. Thus the injective tensor product  $C^\infty(U)_\varepsilon^{\otimes n+1}$  is isomorphic to the projective tensor product  $C^\infty(U)_\gamma^{\otimes n+1}$ . The map

$$f_0 \otimes \dots \otimes f_n \mapsto (x \mapsto f_0(x_0) f_1(x_1) \cdot \dots \cdot f_n(x_n) \in C^\infty(U^{n+1}))$$

is known to extend by continuity to an isomorphism  $C^\infty(U) \otimes_\varepsilon^{n+1} \simeq C^\infty(U^{n+1})$ , hence by nuclearity it also extends to an isomorphism  $C^\infty(U) \otimes_\gamma^{n+1} \simeq C^\infty(U^{n+1})$ . The following commutative diagram summarizes these considerations:

$$\begin{CD} C^\infty(U^{n+1}) @>\Phi_\gamma>> \mathcal{A}_\gamma^{\otimes n+1} \\ @Vj_UVV @VV\text{pr}_\pi^\gamma V \\ C((\text{spec } a)^{n+1}) @>\Phi_\pi>> \mathcal{A}_\pi^{\otimes n+1}. \end{CD}$$

The horizontal arrows are continuous  $*$ -homomorphisms which on elementary tensors are given by  $f_0 \otimes \dots \otimes f_n \mapsto f_0(a) \otimes \dots \otimes f_n(a)$ , the vertical arrows are  $j_U(f) := f|_{(\text{spec } a)^{n+1}} \in C((\text{spec } a)^{n+1})$  resp. the natural map from the projective to the maximal  $C^*$ -tensor product.

**Remark 3.1** (Schwartz functions, entire functions). (1) We note in addition that a functional calculus for, say, Schwartz functions can be set up in a more elementary way by the Fourier transform. Namely, observe that for  $\xi \in \mathbb{R}^{n+1}$  we have

$$\exp(i\xi_0 a^{(0)} + \dots + i\xi_n a^{(n)}) = e^{i\xi_0 a} \otimes e^{i\xi_1 a} \otimes \dots \otimes e^{i\xi_n a},$$

and therefore, since  $\|\cdot\|_\gamma$  is a cross-norm

$$\left\| \exp(i\xi_0 a^{(0)} + \dots + i\xi_n a^{(n)}) \right\|_\gamma = \|e^{i\xi_0 a}\| \cdot \dots \cdot \|e^{i\xi_n a}\| \leq 1.$$

Thus for functions with integrable Fourier transform, e.g. Schwartz functions, we have

$$\Phi_\gamma(f) := f_\gamma(a^{(0)}, \dots, a^{(n)}) = \int_{\mathbb{R}^{n+1}} \widehat{f}(\xi) \exp(i\langle \xi, a^{(j)} \rangle) d\xi, \quad (3.6)$$

where  $\langle \xi, a^{(j)} \rangle$  is an abbreviation for  $\xi_0 a^{(0)} + \dots + \xi_n a^{(n)}$ , and this integral converges in  $\mathcal{A}_\gamma^{\otimes n+1}$  in the Bochner sense.

(2) Finally, for an entire function  $f(z) = \sum_\alpha f_\alpha z^\alpha$  in  $n + 1$  variables  $z = (z_0, \dots, z_n)$ , of course,  $\Phi_\gamma(f) = f_\gamma(a^{(0)}, \dots, a^{(n)})$  is given by the convergent series obtained by inserting  $a^{(j)}$  for  $z_j$ .

**Theorem 3.2.** *Let  $\mathcal{A}$  be a unital  $C^*$ -algebra and let  $a \in \mathcal{A}$  be a selfadjoint element. Furthermore, let  $U \supset \text{spec } a$  be an open neighborhood of  $\text{spec } a$ .*

(1) *There is a unique continuous unital  $*$ -homomorphism  $\Phi_\gamma : C^\infty(U^{n+1}) \simeq C^\infty(U)_\gamma^{\otimes n+1} \rightarrow \mathcal{A}_\gamma^{\otimes n+1}$  sending  $f_0 \otimes \dots \otimes f_n$  to  $f_0(a) \otimes_\gamma \dots \otimes_\gamma f_n(a)$ .  $\Phi_\gamma$  is compatible with the spectral measure of  $a$  in the sense that  $\text{pr}_\pi^\gamma(\Phi_\gamma(f)) = f(a^{(0)}, \dots, a^{(n)})$ . We therefore write  $f_\gamma(a^{(0)}, \dots, a^{(n)})$  for  $\Phi_\gamma(f)$ .*

*For  $f \in C^\infty(U^{n+1})$  the element  $f_\gamma(a^{(0)}, \dots, a^{(n)}) = \Phi_\gamma(f) \in \mathcal{A}_\gamma^{\otimes n+1}$  depends only on  $f$  in an arbitrarily small open neighborhood of  $(\text{spec } a)^{n+1}$ .*

In particular, for  $f$  one may therefore choose a Schwartz function  $\tilde{f}$  with  $\tilde{f} \equiv f$  in such a neighborhood. Then  $f_\gamma(a^{(0)}, \dots, a^{(n)}) = \tilde{f}_\gamma(a^{(0)}, \dots, a^{(n)})$  which can be calculated by the integral Eq. (3.6).

(2) The map

$$C^\infty(U^{n+1}) \times \mathcal{A}_\gamma^{\otimes n} \longrightarrow \mathcal{A},$$

$$(f, b_1 \otimes \cdots \otimes b_n) \mapsto \mu_n(f_\gamma(a^{(0)}, \dots, a^{(n)}) \cdot (b_1 \otimes \cdots \otimes b_n \otimes 1_{\mathcal{A}}))$$

is the unique continuous linear map sending  $(f_0 \otimes \cdots \otimes f_n, b_1 \otimes \cdots \otimes b_n)$  to  $f_0(a) \cdot b_1 \cdot f_1(a) \cdot b_2 \cdot \cdots \cdot b_n \cdot f_n(a)$ .

For the last map we therefore use, as defined in Sec. 3.1.2, the shorthand notation  $f_\gamma(a^{(0)}, \dots, a^{(n)})(b_1 \cdot \cdots \cdot b_n)$ .

*Proof.* This theorem just summarizes what we explained so far in Sec 3.2. The last claim in (1) follows from a simple partition of unity argument.  $\square$

**Remark 3.3.** We note that for a Schwartz function  $f \in \mathcal{S}(\mathbb{R}^{n+1})$  we have as a Bochner integral

$$f_\gamma(a^{(0)}, \dots, a^{(n)})(b_1 \cdot \cdots \cdot b_n) = \int_{\mathbb{R}^{n+1}} \widehat{f}(\xi) \exp_\gamma(i \langle \xi, a^{(\cdot)} \rangle)(b_1 \cdot \cdots \cdot b_n) d\xi$$

$$= \int_{\mathbb{R}^{n+1}} \widehat{f}(\xi) e^{i\xi_0 a} b_1 e^{i\xi_1 a} b_2 \cdot \cdots \cdot b_n e^{i\xi_n a} d\xi,$$

resp. for  $f \in \mathcal{S}(\mathbb{R}^n)$

$$f_\gamma(\nabla_a^{(1)}, \dots, \nabla_a^{(n)})(b_1 \cdot \cdots \cdot b_n) = \int_{\mathbb{R}^n} \widehat{f}(\xi) \exp_\gamma(i \langle \xi, \nabla_a^{(\cdot)} \rangle)(b_1 \cdot \cdots \cdot b_n) d\xi$$

$$= \int_{\mathbb{R}^n} \widehat{f}(\xi) e^{-i\xi_1 a} b_1 e^{i(\xi_1 - \xi_2) a} b_2 \cdot \cdots \cdot b_n e^{i\xi_n a} d\xi.$$

Here we have used

$$i \xi_1 \nabla_a^{(1)} + \cdots + i \xi_n \nabla_a^{(n)} = -i \xi_1 a^{(0)} + i(\xi_1 - \xi_2) a^{(1)} + \cdots + i \xi_n a^{(n)},$$

which follows from Eq. (3.3).

**3.3. The Rearrangement Lemma.** We will need versions of Lemma 2.1 and Theorem 2.2 for the smooth functional calculus in the Banach- $*$ -algebra  $\mathcal{A}_\gamma^{\otimes n+1}$ . For this the integrability conditions Eq. (2.1) and (2.3) have to be assumed for all partial derivatives of the involved function.

**Theorem 3.4** (Smooth Operator Substitution Lemma). *Let  $\mathcal{A}$  be a unital  $C^*$ -algebra and let  $a \in \mathcal{A}$  be a selfadjoint element. Put  $A := e^a$  and let  $U \supset \text{spec } A$  be an open neighborhood of  $\text{spec } A$ .*

(1) Let  $f : \mathbb{R}_{\geq 0} \times U^{n+1} \rightarrow \mathbb{C}$  be a smooth function satisfying the following integrability condition: for each compact subset  $K \subset U$  and each multiindex  $\alpha \in \mathbb{N}^{n+1}$

$$\int_0^\infty \sup_{\lambda \in K} |\partial_\lambda^\alpha f(u, \lambda)| du < \infty. \quad (3.7)$$

Then  $F(\lambda) := \int_0^\infty f(u, \lambda) du$  defines a smooth function on  $U^{n+1}$ , the integral  $\int_0^\infty f_\gamma(u, A^{(0)}, \dots, A^{(n)}) du$  exists as a Bochner integral with values in  $\mathcal{A}_\gamma^{\otimes n+1}$  and the integral equals  $F_\gamma(A^{(0)}, \dots, A^{(n)})$ .

(2) Let  $f : \mathbb{R}_{\geq 0}^{n+1} \rightarrow \mathbb{C}$  be a smooth function such that for each pair of positive real numbers  $0 < C_1 < C_2$  and each multiindex  $\alpha \in \mathbb{N}^{n+1}$

$$\int_0^\infty \sup_{\substack{C_1 \leq s_j \leq C_2 \\ 0 \leq j \leq n}} |u^{|\alpha|} (\partial^\alpha f)(us)| du < \infty. \quad (3.8)$$

Then for the smooth functions

$$F(s) = \int_0^\infty f(u \cdot s) du \quad \text{and} \quad G(\lambda) = \int_0^\infty f(u, u\lambda_1, \dots, u\lambda_n) du$$

as in Theorem 2.2 one has

$$\begin{aligned} \int_0^\infty f_\gamma(uA^{(0)}, \dots, uA^{(n)}) du &= F_\gamma(A^{(0)}, \dots, A^{(n)}) \\ &= A^{-1} G_\gamma(\Delta^{(1)}, \Delta^{(1)} \cdot \Delta^{(2)}, \dots, \Delta^{(1)} \cdot \dots \cdot \Delta^{(n)}) \\ &= A^{-1} \int_0^\infty f_\gamma(u, u\Delta^{(1)}, u\Delta^{(1)} \cdot \Delta^{(2)}, \dots, u\Delta^{(1)} \cdot \dots \cdot \Delta^{(n)}) du. \end{aligned}$$

Both integrals exist in the Bochner sense in  $\mathcal{A}_\gamma^{\otimes n+1}$  resp.  $\mathcal{A}_\gamma^{\otimes n}$ .

*Proof.* (1) The integrability condition guarantees that the integral  $\int_0^\infty f(u, \cdot) du$  converges as a Bochner integral with values in the Fréchet space  $C^\infty(U^{n+1})$ . Thus,  $F$  is smooth and integration commutes with continuous linear maps. Denote by  $\Phi_\gamma$  the  $\mathcal{A}_\gamma^{\otimes n+1}$ -valued spectral measure of  $A^{(0)}, \dots, A^{(n)}$  according to Theorem 3.2. Then

$$\begin{aligned} \int_0^\infty f_\gamma(u, A^{(0)}, \dots, A^{(n)}) du &= \int_0^\infty \Phi_\gamma(f(u, \cdot)) du \\ &= \Phi_\gamma\left(\int_0^\infty f(u, \cdot) du\right) = F_\gamma(A^{(0)}, \dots, A^{(n)}). \end{aligned}$$

(2) Let  $g(u, s) := f(us)$ ,  $h(u, \lambda) := f(u, u\lambda_1, \dots, u\lambda_n)$  as in the proof of Theorem 2.2. Then by the integrability condition the proven first part applies to both functions  $g$  and  $h$  and, taking into account the relations Eq. (3.4), the claim follows as in the proof of Theorem 2.2.  $\square$

Together with Theorem 3.2 we obtain as an immediate consequence:

**Corollary 3.5** (Rearrangement Lemma). *Let  $f_0, \dots, f_p : \mathbb{R}_{\geq 0} \rightarrow \mathbb{C}$  be smooth functions such that  $f(x_0, \dots, x_p) := \prod_{j=0}^p f_j(x_j)$  satisfies the integrability condition Eq. (3.8) of the Smooth Operator Substitution Lemma 3.4. Furthermore, let  $a$  be a selfadjoint element of the unital  $C^*$ -algebra  $\mathcal{A}$ , put  $A := e^a$ . Moreover, denote by  $\Delta^{(\cdot)}, \nabla^{(\cdot)}$  the operators defined in Eq. (3.3). Then for  $b_1, \dots, b_p \in \mathcal{A}$*

$$\begin{aligned} & \int_0^\infty f_0(uA) \cdot b_1 \cdot f_1(uA) \cdot \dots \cdot b_p \cdot f_p(uA) \, du \\ &= A^{-1} \int_0^\infty f_\gamma(u, u\Delta^{(1)}, u\Delta^{(1)}\Delta^{(2)}, \dots, u\Delta^{(1)} \cdot \dots \cdot \Delta^{(p)}) \, du (b_1 \cdot \dots \cdot b_p) \\ &= A^{-1} F_\gamma(\Delta^{(1)}, \Delta^{(1)}\Delta^{(2)}, \dots, \Delta^{(1)} \cdot \dots \cdot \Delta^{(p)})(b_1 \cdot \dots \cdot b_p), \end{aligned} \tag{3.9}$$

where the smooth function  $F(s_1, \dots, s_p)$  is

$$F(s) = \int_0^\infty f_0(u) \cdot f_1(us_1) \cdot \dots \cdot f_p(us_p) \, du.$$

**Example 3.6.** We continue Example 2.4 and put

$$\begin{aligned} f_0(x) &:= x^\nu (1+x)^{-\alpha_0-1}, \\ f_j(x) &:= (1+x)^{-\alpha_j-1}. \end{aligned}$$

Then Corollary 3.5 applies and we recover the Rearrangement Lemma of Connes–Moscovici [3, Lemma 6.2].

**3.4. Noncommutative Taylor expansion in terms of divided differences.** Given selfadjoint elements  $a, b$  of the unital  $C^*$ -algebra  $\mathcal{A}$ . We recast the noncommutative Taylor expansion formula (cf., e.g. [3, Sec. 6.1]) for  $\exp(a+b)$  in light of the functional calculus summarized in Theorem 3.2 and the Genocchi–Hermite formula Eq. (A.3) for divided differences. The main facts about divided differences are summarized in Appendix A below.

The expansional formula for the exponential function reads

$$e^{a+b} = e^a + \sum_{n=1}^\infty \int_{0 \leq s_n \leq \dots \leq s_1 \leq 1} e^{(1-s_1)a} \cdot b \cdot e^{(s_1-s_2)a} \cdot b \cdot \dots \cdot b \cdot e^{s_n a} \, ds. \tag{3.10}$$

The integrand equals, cf. Remark 3.1 and Remark 3.3,

$$\exp_\gamma((1-s_1)a^{(0)} + (s_1-s_2)a^{(1)} + \dots + s_n a^{(n)})(b \cdot \dots \cdot b).$$

Applying the Genocchi–Hermite formula Eq. (A.3) to the exponential function we have

$$\int_{0 \leq s_n \leq \dots \leq s_1 \leq 1} \exp_\gamma \left( (1 - s_1)a^{(0)} + (s_1 - s_2)a^{(1)} + \dots + s_n a^{(n)} \right) ds_1 \dots ds_n = [a^{(0)}, \dots, a^{(n)}] \exp_\gamma .$$

In other words the general term in the expansion formula Eq. (3.10) can be reinterpreted as follows: take the commuting selfadjoint operators  $a^{(0)}, \dots, a^{(n)}$  and insert them into the multivariable function  $x \mapsto [x_0, \dots, x_n] \exp$ , the  $n^{\text{th}}$  divided difference of the exponential function. Then contract with the  $n$ -fold tensor product  $b \otimes \dots \otimes b$ .

Therefore, the formula Eq. (3.10) may be rewritten in the very compact way

$$e^{a+b} = \sum_{n=0}^{\infty} ([a^{(0)}, \dots, a^{(n)}] \exp_\gamma)(b \cdot \dots \cdot b) \tag{3.11}$$

$$= \sum_{n=0}^{\infty} e^a ([0, \nabla_a^{(1)}, \nabla_a^{(1)} + \nabla_a^{(2)}, \dots, \nabla_a^{(1)} + \dots + \nabla_a^{(n)}] \exp_\gamma)(b \cdot \dots \cdot b). \tag{3.12}$$

In the second line we have used the functional equation of  $\exp$ , the homogeneity of the divided differences (cf. Eq. (A.1)), and the relations Eq. (3.5). In a different context it was also observed in [1] that the expansion formula Eq. (3.10) can be interpreted in terms of the Genocchi–Hermite formula. We obtain a straightforward generalization of Eq. (3.11), (3.12) to arbitrary smooth functions.

**Proposition 3.7.** *Let  $a \in \mathcal{A}$  be selfadjoint. Then for a smooth function  $f$  in a neighborhood of  $\text{spec } a$  the Taylor expansion of  $f(a + b)$  for selfadjoint  $b \sim 0$  is given by*

$$f(a + b) \sim_{b \rightarrow 0} \sum_{n=0}^{\infty} ([a^{(0)}, \dots, a^{(n)}] f_\gamma)(b \cdot \dots \cdot b).$$

**Remark 3.8.** (1) Note that if  $\mathcal{A} = \mathbb{C}$  and hence  $a, b$  are real numbers then  $\mathcal{A}^{\otimes n+1}$  is canonically isomorphic to  $\mathbb{C}$  and under this isomorphism  $([a^{(0)}, \dots, a^{(n)}] f_\gamma) \cdot (b \cdot \dots \cdot b)$  corresponds to  $\frac{1}{n!} f^{(n)}(a) b^n$ , see Eq. (A.5), and the proposition just gives the ordinary Taylor formula.

(2) The formula in Prop. 3.7 is equivalent to the noncommutative Taylor expansion formula derived in [15] in the context of formal power series. This expansion was in fact discovered earlier by Daletskii [5]. We plan to discuss such expansions and its relations to a noncommutative Newton interpolation formula in more detail in the near future.

*Proof.* W. l. o. g. we may assume that  $f$  is a Schwartz function on  $\mathbb{R}$ , cf. Theorem 3.2(1). Write

$$f(a+b) = \int_{\mathbb{R}} \widehat{f}(\xi) e^{i\xi(a+b)} d\xi.$$

Then apply the expansion formula Eq. (3.10) to the exponential term

$$e^{i\xi(a+b)} = e^{i\xi a} + \sum_{n=1}^{\infty} (i\xi)^n ([i\xi a^{(0)}, \dots, i\xi a^{(n)}] \exp_{\gamma})(b \cdot \dots \cdot b).$$

Noting that  $(i\xi)^n \widehat{f}(\xi) = \widehat{f^{(n)}}(\xi)$  the  $n$ -th term (with the  $b$ 's omitted) equals

$$\int_{0 \leq s_n \leq \dots \leq s_1 \leq 1} f_{\gamma}^{(n)}((1-s_1)a^{(0)} + (s_1-s_2)a^{(1)} + \dots + s_n a^{(n)}) ds_1 \dots ds_n = [a^{(0)}, \dots, a^{(n)}] f_{\gamma},$$

where Genocchi–Hermite's formula Eq. (A.3) was used.  $\square$

**Example 3.9.** Let  $a(s, t) \in \mathcal{A}$  be a smooth selfadjoint family with  $a(0, 0) = a$ . Put  $\delta_1 a := \partial_s|_{s=0} a(s, 0)$ ,  $\delta_2 a := \partial_t|_{t=0} a(0, t)$ , and  $\delta_1 \delta_2 a := \partial_s \partial_t|_{s=t=0} a(s, t)$ . Then

$$\partial_s|_{s=0} f(a(s, 0)) = ([a^{(0)}, a^{(1)}] f_{\gamma})(\delta_1 a), \quad (3.13)$$

$$\begin{aligned} \partial_s \partial_t|_{s=t=0} f(a(s, t)) &= ([a^{(0)}, a^{(1)}] f_{\gamma})(\delta_1 \delta_2 a) \\ &\quad + ([a^{(0)}, a^{(1)}, a^{(2)}] f_{\gamma})(\delta_1 a \delta_2 a + \delta_2 a \delta_1 a). \end{aligned} \quad (3.14)$$

Taking into account Eq. (3.12) we obtain for the exponential function

$$e^{-a} \partial_s|_{s=0} e^{a(s, 0)} = ([0, \nabla_a^{(1)}] \exp_{\gamma})(\delta_1 a), \quad (3.15)$$

$$\begin{aligned} e^{-a} \partial_s \partial_t|_{s=t=0} e^{a(s, t)} &= ([0, \nabla_a^{(1)}] \exp_{\gamma})(\delta_1 \delta_2 a) \\ &\quad + ([0, \nabla_a^{(1)}, \nabla_a^{(1)} + \nabla_a^{(2)}] \exp_{\gamma})(\delta_1 a \delta_2 a + \delta_2 a \delta_1 a). \end{aligned} \quad (3.16)$$

Note that

$$[0, s] \exp = \frac{e^s - 1}{s}, \quad (3.17)$$

$$[0, s, s+t] \exp = \frac{e^{s+t} s + t - e^s (s+t)}{st(s+t)}. \quad (3.18)$$

One should compare this to [4, (21)], [3, (167)–(169)], and [8, Lemma 5.1].

**3.5. Expansion formulas for  $\nabla_a$ .** Recall from Eq. (3.3)  $\nabla_a := \nabla_a^{(1)} = -a \otimes 1_{\mathcal{A}} + 1_{\mathcal{A}} \otimes a \in \mathcal{A} \otimes \mathcal{A}$ . To expand  $f(\nabla_{a+b})$  we therefore have to apply the expansion of Proposition 3.7 in the algebra  $\tilde{\mathcal{A}} := \mathcal{A} \otimes_{\gamma} \mathcal{A}$ . Denote for  $c \in \tilde{\mathcal{A}}$ , analogously to Eq. (3.3),

$$\begin{aligned} \tilde{c}^{(j)} &= (1_{\tilde{\mathcal{A}}}, \dots, 1_{\tilde{\mathcal{A}}}, c, 1_{\tilde{\mathcal{A}}}, \dots, 1_{\tilde{\mathcal{A}}}), \quad 0 \leq j \leq n \quad (c \text{ is in the } j\text{-th slot}), \\ \tilde{\nabla}_a^{(j)} &:= (\nabla_a)^{(j)} = (1_{\tilde{\mathcal{A}}}, \dots, 1_{\tilde{\mathcal{A}}}, \nabla_a, 1_{\tilde{\mathcal{A}}}, \dots, 1_{\tilde{\mathcal{A}}}), \quad 0 \leq j \leq n. \end{aligned}$$

**Lemma 3.10.** *Let  $f \in \mathcal{S}(\mathbb{R}^{n+1})$  be a Schwartz function, let  $b'_j \otimes b''_j \in \tilde{\mathcal{A}}$ ,  $j = 1, \dots, n$ , and let  $x \in \mathcal{A}$  be given. Note that  $f_{\gamma}(\tilde{\nabla}_a^{(0)}, \dots, \tilde{\nabla}_a^{(n)}) \in \tilde{\mathcal{A}}^{\otimes n+1}$ . After contraction with  $(b'_1 \otimes b''_1) \otimes \dots \otimes (b'_n \otimes b''_n)$  one obtains an element of  $\mathcal{A}$  which can be contracted further with  $x \in \mathcal{A}$  to an element of  $\mathcal{A}$ . For this element we have*

$$\begin{aligned} &(f_{\gamma}(\tilde{\nabla}_a^{(0)}, \dots, \tilde{\nabla}_a^{(n)})(b'_1 \otimes b''_1 \cdot \dots \cdot b'_n \otimes b''_n))(x) \\ &= f_{\gamma}(-a^{(0)} + a^{(n+1)}, -a^{(1)} + a^{(n+2)}, \dots, -a^{(n)} + a^{(2n+1)}) \\ &\quad (b'_1 \cdot \dots \cdot b'_n \cdot x \cdot b''_1 \cdot \dots \cdot b''_n) \\ &= f_{\gamma}(\nabla_a^{(1)} + \dots + \nabla_a^{(n+1)}, \nabla_a^{(2)} + \dots + \nabla_a^{(n+2)}, \dots, \nabla_a^{(n+1)} + \dots + \nabla_a^{(2n+1)}) \\ &\quad (b'_1 \cdot \dots \cdot b'_n \cdot x \cdot b''_1 \cdot \dots \cdot b''_n). \end{aligned}$$

*Proof.* This follows from a straightforward calculation:

$$\begin{aligned} &(f_{\gamma}(\tilde{\nabla}_a^{(0)}, \dots, \tilde{\nabla}_a^{(n)})(b'_1 \otimes b''_1 \cdot \dots \cdot b'_n \otimes b''_n))(x) \\ &= \int_{\mathbb{R}^{n+1}} \hat{f}(\xi) (e^{-i\xi_0 a} \otimes e^{i\xi_0 a} b'_1 \otimes b''_1 \otimes \dots \otimes b'_n \otimes b''_n e^{-i\xi_n a} \otimes e^{i\xi_n a})(x) d\xi \\ &= \int_{\mathbb{R}^{n+1}} \hat{f}(\xi) e^{-i\xi_0 a} b'_1 e^{-i\xi_1 a} b'_2 \cdot \dots \cdot b'_n e^{-i\xi_n a} x e^{i\xi_0 a} b''_1 \cdot \dots \cdot b''_n e^{i\xi_n a} d\xi \\ &= f_{\gamma}(-a^{(0)} + a^{(n+1)}, -a^{(1)} + a^{(n+2)}, \dots, -a^{(n)} + a^{(2n+1)}) \\ &\quad (b'_1 \cdot \dots \cdot b'_n \cdot x \cdot b''_1 \cdot \dots \cdot b''_n). \quad \square \end{aligned}$$

This Lemma and the expansion 3.7 allow to expand  $f(\nabla_{a+b})(x)$  in principle to any order, although the combinatorics becomes tedious. We note the expansion up to order 2, cf. [3, Lemma 4.11 and Lemma 4.12].

**Proposition 3.11.** *Let  $a, x \in \mathcal{A}$  be selfadjoint. Then for a Schwartz function  $f \in \mathcal{S}(\mathbb{R})$  the Taylor expansion up to order 2 of  $f(\nabla_{a+b})(x)$  for selfadjoint  $b \sim 0$*

is given by

$$\begin{aligned}
f(\nabla_{a+b})(x) &= f(\nabla_a)(x) \\
&\quad - ([\nabla_a^{(1)} + \nabla_a^{(2)}, \nabla_a^{(2)}]f_\gamma)(b \cdot x) + ([\nabla_a^{(1)} + \nabla_a^{(2)}, \nabla_a^{(1)}]f_\gamma)(x \cdot b) \\
&\quad + ([\nabla_a^{(1)} + \nabla_a^{(2)} + \nabla_a^{(3)}, \nabla_a^{(2)} + \nabla_a^{(3)}, \nabla_a^{(3)}]f_\gamma)(b \cdot b \cdot x) \\
&\quad + ([\nabla_a^{(1)}, \nabla_a^{(1)} + \nabla_a^{(2)}, \nabla_a^{(1)} + \nabla_a^{(2)} + \nabla_a^{(3)}]f_\gamma)(x \cdot b \cdot b) \\
&\quad + ([\nabla_a^{(1)} + \nabla_a^{(2)}, \nabla_a^{(1)} + \nabla_a^{(2)} + \nabla_a^{(3)}, \nabla_a^{(2)} + \nabla_a^{(3)}]f_\gamma)(b \cdot x \cdot b) \\
&\quad + ([\nabla_a^{(1)} + \nabla_a^{(2)}, \nabla_a^{(2)}, \nabla_a^{(2)} + \nabla_a^{(3)}]f_\gamma)(b \cdot x \cdot b).
\end{aligned}$$

The two variable functions involved in the linear term are

$$-[s+t, t]f = -\frac{f(s+t) - f(t)}{s}, \quad [s+t, s]f = \frac{f(s+t) - f(s)}{t}, \quad (3.19)$$

this should be compared to [3, (134)].

*Proof.* One just has to apply Prop. 3.7 to  $f(\nabla_{a+b})$  in the algebra  $\tilde{\mathcal{A}}$  and apply the previous Lemma. We do the calculation for the linear term and leave the second order term to the interested reader.

$$\begin{aligned}
([\tilde{\nabla}_a^{(0)}, \tilde{\nabla}_a^{(1)}]f_\gamma)(\tilde{\nabla}_b)(x) &= ([\tilde{\nabla}_a^{(0)}, \tilde{\nabla}_a^{(1)}]f_\gamma)(-b \otimes 1_{\tilde{\mathcal{A}}} + 1_{\tilde{\mathcal{A}}} \otimes b)(x) \\
&= ([-a^{(0)} + a^{(2)}, -a^{(1)} + a^{(3)}]f_\gamma)(-b \cdot x \cdot 1 + 1 \cdot x \cdot b) \\
&= -([\nabla_a^{(1)} + \nabla_a^{(2)}, \nabla_a^{(2)}]f_\gamma)(b \cdot x) \\
&\quad + ([\nabla_a^{(1)} + \nabla_a^{(2)}, \nabla_a^{(1)}]f_\gamma)(x \cdot b). \quad \square
\end{aligned}$$

**Corollary 3.12.** *Let  $\varphi$  be a tracial state on  $\mathcal{A}$ . Then, for selfadjoint elements  $a, b, x, y \in \mathcal{A}$  we have*

$$\begin{aligned}
\frac{d}{d\varepsilon} \Big|_{\varepsilon=0} \varphi(f(\nabla_{a+\varepsilon b})(x)y) \\
= -\varphi(b([\nabla_a^{(1)}, -\nabla_a^{(2)}]f_\gamma)(x \cdot y)) + \varphi(b([\nabla_a^{(1)}, \nabla_a^{(2)}]f_\gamma)(y \cdot x)).
\end{aligned}$$

Note that

$$-[s, -t]f = \frac{f(-t) - f(s)}{s+t}, \quad [-s, t]f = \frac{f(t) - f(-s)}{s+t}. \quad (3.20)$$

This should be compared to [3, (131)], where  $f$  is assumed to be even and hence  $-[s, -t]f = [-s, t]f = \frac{f(t) - f(s)}{s+t}$ .

*Proof.* Using the previous proposition we calculate

$$\begin{aligned} \frac{d}{d\varepsilon} \Big|_{\varepsilon=0} \varphi(f(\nabla_{a+\varepsilon b})(x)y) &= -\varphi([-a^{(0)} + a^{(2)}, -a^{(1)} + a^{(2)}]f_\gamma)(b \cdot x \cdot y) \\ &\quad + \varphi([-a^{(0)} + a^{(2)}, -a^{(0)} + a^{(1)}]f_\gamma)(x \cdot b \cdot y) \\ &= -\varphi(b([-a^{(2)} + a^{(1)}, -a^{(0)} + a^{(1)}]f_\gamma)(x \cdot y)) \\ &\quad + \varphi(b([-a^{(1)} + a^{(0)}, -a^{(1)} + a^{(2)}]f_\gamma)(y \cdot x)), \end{aligned}$$

and the result follows in view of Eq. (3.3) and the fact that divided differences are symmetric functions of their arguments.  $\square$

#### 4. The functions occurring in the Rearrangement Lemma for the modular curvature

**4.1. The Mellin transform of  $(1+x)^{-m-1}$ .** By a contour integral argument [19, 3.123] the Mellin transform of  $x \mapsto (1+x)^{-1}$  is given by

$$\int_0^\infty x^{z-1} \frac{1}{1+x} dx = \frac{\pi}{\sin \pi z}, \quad 0 < \Re z < 1,$$

and integration by parts yields

$$\int_0^\infty x^{z-1} \frac{1}{(1+x)^{m+1}} dx = \frac{(z-1)^m}{m!} \frac{\pi}{\sin \pi z}.$$

Since  $\frac{1}{\sin \pi z}$  decays exponentially on vertical lines we conclude that the functions  $x \mapsto (1+x)^{-m-1}$  are given by the inversion formula

$$(1+x)^{-m-1} = \int_{\Re z = \alpha} x^{-z} \frac{(z-1)^m}{m!} \frac{\pi}{\sin \pi z} dz$$

for  $0 < \Re \alpha < 1$ .

**4.2. The functions  $M_\alpha^{(p)}(s, m)$  and  $H_\alpha^{(p)}(s, m)$ .** Given  $p \in \mathbb{Z}_{\geq 1}$ , a multiindex  $\alpha \in \mathbb{N}^{p+1}$  and  $s_j > 0, j = 0, \dots, p$ , put

$$M_\alpha^{(p)}(s, z) := \int_0^\infty x^{|\alpha|+p-1-z} \cdot \prod_{j=0}^p (1+s_j x)^{-\alpha_j-1} dx, \quad -1 < \Re z < |\alpha| + p, \quad (4.1)$$

$$= \int_0^\infty x^z \cdot \prod_{j=0}^p (x+s_j)^{-\alpha_j-1} dx, \quad (4.2)$$

where the second line is obtained by changing variables  $x \mapsto x^{-1}$ . Furthermore,

$$H_\alpha^{(p)}(s', z) := M_\alpha^{(p)}((1, s'), z), \quad s' = (s_1, \dots, s_p).$$

We are mainly interested in integral values of  $z$ . The integrals Eq. (4.1), (4.2) converge absolutely for  $-1 < \Re z < |\alpha| + p$ . So  $z = m \in \mathbb{Z}$  may take the values  $0, 1, \dots, |\alpha| + p - 1$ . The function  $M_\alpha^{(p)}(\cdot, z)$  is  $(-|\alpha| - p + z)$ -homogeneous, that is

$$M_\alpha^{(p)}(\lambda s, z) = \lambda^{-|\alpha| - p + z} M_\alpha^{(p)}(s, z), \quad (4.3)$$

as is seen by changing variables from  $\lambda x$  to  $x$ . Therefore, scaling  $s_0$  gives

$$M_\alpha^{(p)}(s, z) = s_0^{-|\alpha| - p + z} H_\alpha^{(p)}(s'/s_0, z).$$

$M_\alpha^{(p)}(s, m)$  and  $H_\alpha^{(p)}(s, m)$  can be expressed in terms of closed formulas involving divided differences and differentiations:

**Proposition 4.1.** *For a multiindex  $\alpha = (\alpha_0, \dots, \alpha_p) \in \mathbb{N}^{p+1}$  and  $s = (s_0, \dots, s_p)$  with  $s_j > 0$  let  $(u_0, \dots, u_{|\alpha|+p})$  be the tuple with  $u_0 = \dots = u_{\alpha_0} = s_0, u_{\alpha_0+1} = \dots = u_{\alpha_0+\alpha_1+1} = s_1, \dots, u_{|\alpha|+p-1-\alpha_p} = \dots = u_{|\alpha|+p} = s_p$ .<sup>4</sup> Furthermore, let  $\alpha' := (0, \alpha_1, \dots, \alpha_p)$ . Then for  $m \in \{0, 1, \dots, |\alpha| + p - 1\}$*

$$M_\alpha^{(p)}(s, m) = (-1)^{m+|\alpha|+p-1} [u_0, \dots, u_{|\alpha|+p}] \text{id}^m \log \quad (4.4)$$

$$= \frac{(-1)^{m+|\alpha|+p-1}}{\alpha!} \partial_s^\alpha [s_0, \dots, s_p] \text{id}^m \log. \quad (4.5)$$

Here,  $\text{id}^m$  stands for the function  $x \mapsto x^m$  and  $[y_0, \dots, y_n]f$  stands for the divided difference of the function  $f$  with respect to the variables  $y_0, \dots, y_n$ .

If  $m \in \{0, 1, \dots, |\alpha'| + p - 1\}$  then also

$$M_\alpha^{(p)}(s, m) = \frac{(-1)^{|\alpha'|+p-1-m}}{\alpha!} \left( \sum_{k=1}^p s_k \partial_{s_k} + |\alpha| + p - 1 - m \right)^{\alpha_0} \cdot \partial_s^{\alpha'} [s_0, \dots, s_p] \text{id}^m \log. \quad (4.6)$$

Here,  $(\sum_{k=1}^p s_k \partial_{s_k} + |\alpha| + p - 1 - m)^{\alpha_0}$  is the differential operator  $\sum_{k=1}^p s_k \partial_{s_k} + |\alpha| + p - 1 - m$  inserted into the falling factorial polynomial  $(a)^{\alpha_0} = a \cdot (a-1) \cdot \dots \cdot (a - \alpha_0 + 1)$ .

Consequently, for  $H_\alpha^{(p)}$  and  $m \in \{0, 1, \dots, |\alpha'| + p - 1\}$  we have the following formula which only involves partial derivatives in the variables  $s_1, \dots, s_p$

$$\begin{aligned} H_\alpha^{(p)}(s', m) &= M_\alpha^{(p)}((1, s'), m), \quad s' = (s_1, \dots, s_p) \\ &= \frac{(-1)^{|\alpha'|+p-1-m}}{\alpha!} \left( \sum_{k=1}^p s_k \partial_{s_k} + |\alpha| + p - 1 - m \right)^{\alpha_0} \\ &\quad \cdot \partial_s^{\alpha'} [1, s_1, \dots, s_p] \text{id}^m \log. \end{aligned} \quad (4.7)$$

<sup>4</sup>In other words, the tuple  $u$  consists of  $\alpha_0 + 1$  copies of  $s_0$ ,  $\alpha_1 + 1$  copies of  $s_1$  etc.

Recall that divided differences are explained in Appendix A below. For more on the falling factorials see Sec. B.1 below.

*Proof.* We start with distinct positive variables  $t_0, \dots, t_q; q := |\alpha| + p$ . Then by Eq. (4.2)

$$M_0^{(q)}(t, m) = \int_0^\infty x^m \prod_{j=0}^q (x + t_j)^{-1} dx.$$

The integrand is a rational function of degree  $m - q - 1 \leq -2$ . Therefore, it has a partial fraction decomposition

$$x^m \prod_{j=0}^q (x + t_j)^{-1} = \sum_{k=0}^q A_k (x + t_k)^{-1},$$

with  $\sum_{k=0}^q A_k = 0$ . The  $A_k$  are explicitly given by

$$A_k = (-t_k)^m \prod_{j=0, j \neq k}^q (t_j - t_k)^{-1} = (-1)^{m+q} t_k^m \prod_{j=0, j \neq k}^q (t_k - t_j)^{-1}.$$

Thus we find

$$\begin{aligned} M_0^{(q)}(t, m) &= - \sum_{k=0}^q A_k \log t_k \\ &= (-1)^{m+q-1} \sum_{k=0}^q \left( \prod_{j=0, j \neq k}^q (t_k - t_j)^{-1} \right) t_k^m \log t_k \quad (4.8) \\ &= (-1)^{m+q-1} [t_0, \dots, t_q] \text{id}^m \log. \end{aligned}$$

In the last equation Eq. (A.2) was used. By continuity this formula also holds for not necessarily distinct variables  $t_0, \dots, t_q$ . Hence by Eq. (A.5)

$$\begin{aligned} M_\alpha^{(p)}(s, m) &= (-1)^{m+|\alpha|+p-1} [s_0^{\alpha_0+1}, \dots, s_p^{\alpha_p+1}] \text{id}^m \log \\ &= \frac{(-1)^{m+|\alpha|+p-1}}{\alpha!} \partial_s^\alpha [s_0, \dots, s_p] \text{id}^m \log, \end{aligned}$$

thus Eq. (4.4) and Eq. (4.5) are proved.

The proof of the remaining claims about the formulas involving falling factorials is postponed to the Appendix B.  $\square$

**Remark 4.2.** For general  $z \notin \mathbb{Z}$  one may calculate  $M_0^{(q)}(t, z)$  similarly. From the partial fraction decomposition

$$\prod_{j=0}^q (x + t_j)^{-1} = \sum_{k=0}^q A_k (x + t_k)^{-1},$$

$$A_k = (-1)^q \prod_{j=0, j \neq k}^q (t_k - t_j)^{-1},$$

and Sec. 4.1 we infer

$$\begin{aligned} M_0^{(q)}(t, z) &= \frac{-\pi}{\sin \pi z} \sum_{k=0}^q A_k t_k^z \\ &= \frac{(-1)^{q-1} \pi}{\sin \pi z} \sum_{k=0}^q \left( \prod_{j=0, j \neq k}^q (t_k - t_j)^{-1} \right) t_k^z \\ &= \frac{(-1)^{q-1} \pi}{\sin \pi z} [t_0, \dots, t_q] \text{id}^z. \end{aligned}$$

Taking the limit  $z \rightarrow m \in \mathbb{Z}$  one obtains again Eq. (4.8).

## 5. Examples

Recall from Eq. (4.1), (4.2) and Proposition 4.1 that for  $s_j > 0$  and  $m \in \{0, 1, \dots, |\alpha| + p - 1\}$

$$H_\alpha^{(p)}(s, m) := \int_0^\infty x^{|\alpha|+p-1-m} \cdot (1+x)^{-\alpha_0-1} \cdot \prod_{j=1}^p (1+s_j x)^{-\alpha_j-1} dx, \quad (5.1)$$

$$= \int_0^\infty x^m \cdot (1+x)^{-\alpha_0-1} \cdot \prod_{j=1}^p (x+s_j)^{-\alpha_j-1} dx \quad (5.2)$$

$$= (-1)^{m+|\alpha|+p-1} \cdot [1^{\alpha_0+1}, s_1^{\alpha_1+1}, \dots, s_p^{\alpha_p+1}] \text{id}^m \log. \quad (5.3)$$

The recursion formula Eq. (A.1), the Leibniz rule Eq. (A.6), and the substitution rule Eq. (A.7) lead to a large variety of recursion formulas for the functions  $H_\alpha^{(p)}$ . We will discuss here the case of one and two variable functions and in particular compare the two variable case to the examples listed at the end of [3].

**5.1. One variable functions.**

**5.1.1.** From Eq. (4.7) we infer

$$H_{0,0}^{(1)}(s) := H_{0,0}^{(1)}(s, 0) := [1, s] \log = \frac{\log s}{s-1} =: \mathcal{L}_0(s). \tag{5.4}$$

Note that if we substitute  $s = \exp(u)$  this function becomes

$$\frac{u}{e^u - 1} = \sum_{j=0}^{\infty} \frac{B_j}{j!} u^j, \tag{5.5}$$

which is the generating function for the Bernoulli numbers. The fact that by Proposition 4.1 all the functions  $H_{\alpha}^{(p)}$  are ultimately expressed in terms of the function  $\frac{\log s}{s-1}$  is one of the “conceptual explanations” the formidable formulas (3) and (4) in [3] are “begging” for.

Applying Proposition 4.1 we find if  $m \in \{0, 1, \dots, \alpha_1\}$

$$H_{\alpha}^{(1)}(s, m) = \frac{(-1)^{|\alpha_1|+m}}{\alpha!} (D_s + |\alpha| - m)^{\alpha_0} \partial_s^{\alpha_1} \frac{s^m \log s}{s-1} \tag{5.6}$$

$$= \frac{(-1)^{\alpha_1+m}}{\alpha!} s^{m-\alpha_1} \partial_s^{\alpha_0} s^{|\alpha|-m} \partial_s^{\alpha_1} \frac{s^m \log s}{s-1} \tag{5.7}$$

$$= \frac{(-1)^{\alpha_1+m}}{\alpha!} \partial_s^{\alpha_1} s^m \partial_s^{\alpha_0} \frac{s^{\alpha_0} \log s}{s-1}, \tag{5.8}$$

resp. for  $m = 0$

$$H_{\alpha}^{(1)}(s) := H_{\alpha}^{(1)}(s, 0) = (-1)^{|\alpha|} [1^{\alpha_0+1}, s^{\alpha_1+1}] \log \tag{5.9}$$

$$= (-1)^{|\alpha|} [1^{\alpha_0}, s^{\alpha_1+1}] \mathcal{L}_0, \quad \mathcal{L}_0(s) := [1, s] \log \tag{5.10}$$

$$= \frac{(-1)^{\alpha_1}}{\alpha!} s^{-\alpha_1} \partial_s^{\alpha_0} s^{|\alpha|} \partial_s^{\alpha_1} \frac{\log s}{s-1} \tag{5.11}$$

$$= \frac{(-1)^{\alpha_1}}{\alpha!} \partial_s^{|\alpha|} \frac{s^{\alpha_0} \log s}{s-1}, \tag{5.12}$$

where the substitution rule Eq. (A.7) was used. For the equalities Eq. (5.8) and (5.12) cf. Eq. (B.3).

**5.1.2.** We note the special case

$$\begin{aligned} \mathcal{L}_m(s) &:= H_{0,m}^{(1)}(s, m) = H_{m,0}^{(1)}(s, 0) = (-1)^m [1^{m+1}, s] \log \\ &= (-1)^m [1^m, s] \mathcal{L}_0 = \frac{1}{m!} \partial_s^m \frac{s^m \log s}{s-1} \\ &= \frac{(-1)^m}{(s-1)^{m+1}} \left( \log s - \sum_{j=1}^m \frac{(-1)^{j-1}}{j} (s-1)^j \right) \end{aligned} \tag{5.13}$$

which was called “modified Logarithm” in [4, Sec. 3 and 6].

We list the first few functions explicitly.

$$\begin{aligned}
H_{1,0}^{(1)}(s) &= \mathcal{L}_1(s) = -[1, s]\mathcal{L}_0 = -\frac{\log s - s + 1}{(s-1)^2}, \\
H_{0,1}^{(1)}(s) &= \frac{s \log s - s + 1}{s(s-1)^2}, \\
H_{1,1}^{(1)}(s) &= [1^2, s^2] \log = -\partial_s H_{1,0}^{(1)}(s) = -\frac{2s \log s - s^2 + 1}{(s-1)^3 s}.
\end{aligned} \tag{5.14}$$

**5.2. Two variable functions.** Instead of the clumsy  $H_\alpha^{(2)}((a, b), 0)$  we write  $H_\alpha^{(2)}(a, b)$ . By Eq. (4.7) and the substitution rule Eq. (A.7) we have

$$\begin{aligned}
H_\alpha^{(2)}(a, b) &= (-1)^{|\alpha|+1} [1^{\alpha_0+1}, a^{\alpha_1+1}, b^{\alpha_2+1}] \log, \\
&= (-1)^{|\alpha|+1} [1^{\alpha_0}, a^{\alpha_1+1}, b^{\alpha_2+1}] \mathcal{L}_0 \\
&= (-1)^{|\alpha|+1} \frac{1}{b-a} \left( [1^{\alpha_0}, a^{\alpha_1}, b^{\alpha_2+1}] \mathcal{L}_0 - [1^{\alpha_0}, a^{\alpha_1+1}, b^{\alpha_2}] \mathcal{L}_0 \right) \\
&= \frac{(-1)^{|\alpha|+\alpha_0+1}}{\alpha_1! \alpha_2!} \partial_a^{\alpha_1} \partial_b^{\alpha_2} \frac{1}{b-a} \left( \mathcal{L}_{\alpha_0}(b) - \mathcal{L}_{\alpha_0}(a) \right).
\end{aligned} \tag{5.15}$$

Thus in the special case  $\alpha_1 = \alpha_2 = 0$  we immediately obtain a simple formula expressing two variable functions in terms of one variable modified logarithms:

$$H_{r,0,0}^{(2)}(a, b) = \frac{-1}{b-a} (\mathcal{L}_r(b) - \mathcal{L}_r(a)). \tag{5.16}$$

**5.3. Comparison with the explicit formulas in [3].** For two variable functions  $H_\alpha^{(2)}(s)$  let us compare our results to the explicit formulas given at the end of [3]. We denote the function  $H$  introduced there by  $H^{CM}$ . Then for the two variable functions we have by definition  $H_{\alpha_0+1, \alpha_1+1, \alpha_2+1}^{CM}(a, b) = H_\alpha^{(2)}(a, b)$ .

In [3] the following formulas are given explicitly. In the resp. first lines we list the formulas as stated in loc. cit., in the resp. second lines we cancel common factors and write them as a sum of fractions involving  $\log(a)$ ,  $\log(b)$  plus terms which do not contain logarithms. As a helper the open source computer algebra system Maxima was used.

$$\begin{aligned}
H_{1,1,1}^{CM}(a, b) &= \frac{(-1+b)\log(a) - (-1+a)\log(b)}{(-1+a)(-1+b)(-a+b)} \\
&= \frac{\log(a)}{(a-1)(b-a)} - \frac{\log(b)}{(b-1)(b-a)}, \\
H_{1,2,1}^{CM}(a, b) &= \frac{(-1+b)((-1+a)(a-b) + a(1-2a+b)\log(a)) + (-1+a)^2 a \log(b)}{(-1+a)^2 a (a-b)^2 (-1+b)} \\
&= \frac{(b-2a+1)\log(a)}{(a-1)^2 (b-a)^2} + \frac{\log(b)}{(b-1)(b-a)^2} - \frac{1}{(b-a)(a-1)a},
\end{aligned}$$

$$\begin{aligned}
H_{2,1,1}^{CM}(a, b) &= \frac{(-1+b)^2 \log(a) + (-1+a)((a-b)(-1+b) - (-1+a)\log(b))}{(-1+a)^2(a-b)(-1+b)^2} \\
&= -\frac{\log(a)}{(b-a)(a-1)^2} + \frac{\log(b)}{(b-1)^2(b-a)} + \frac{1}{(b-1)(a-1)}, \\
H_{2,2,1}^{CM}(a, b) &= \frac{(-1+b)((-1+a)(a-b)(1+a^2 - (1+a)b) + a(-1+3a-2b)(-1+b)\log(a)) - (-1+a)^3 a \log(b)}{(-1+a)^3 a(a-b)^2(-1+b)^2} \\
&= -\frac{(2b-3a+1)\log(a)}{(b-a)^2(a-1)^3} - \frac{\log(b)}{(b-1)^2(b-a)^2} + \frac{(a+1)b - a^2 - 1}{(b-1)(b-a)(a-1)^2 a}, \\
H_{3,1,1}^{CM}(a, b) &= \frac{(-1+a)(5+a(-3+b) - 3b)(a-b)(-1+b) - 2(-1+b)^3 \log(a) + 2(-1+a)^3 \log(b)}{2(-1+a)^3(a-b)(-1+b)^3} \\
&= \frac{\log(a)}{(b-a)(a-1)^3} - \frac{\log(b)}{(b-a)(b-1)^3} + \frac{(a-3)b - 3a + 5}{2(b-1)^2(a-1)^2}.
\end{aligned}$$

From the resp. second lines we see immediately that  $H_{1,1,1}^{CM}(a, b) = -[1, a, b] \log$  and that  $H_{1,2,1}^{CM}(a, b) = -\partial_a H_{1,1,1}^{CM}(a, b)$ .

To  $H_{2,1,1}^{CM}$  and  $H_{3,1,1}^{CM}$  we can apply Eq. (5.16) and obtain

$$\begin{aligned}
H_{2,1,1}^{CM}(a, b) &= \frac{-1}{b-a} (\mathcal{L}_1(b) - \mathcal{L}_1(a)), \\
H_{3,1,1}^{CM}(a, b) &= \frac{-1}{b-a} (\mathcal{L}_2(b) - \mathcal{L}_2(a)).
\end{aligned}$$

Alternatively, one may employ the formulas in Proposition 4.1 and indeed one verifies

$$\begin{aligned}
H_{2,1,1}^{CM}(a, b) &= \partial_s \Big|_{s=1} [s, a, b] \log \\
&= -(a\partial_a + b\partial_b + 2)[1, a, b] \log \\
&= (a\partial_a + b\partial_b + 2)H_{1,1,1}^{CM}(a, b), \\
H_{3,1,1}^{CM}(a, b) &= H_{2,0,0}^{(2)}(a, b) = -\frac{1}{2}(a\partial_a + b\partial_b + 3)^2 [1, a, b] \log \\
&= -\frac{1}{2}(a\partial_a + b\partial_b + 3)(a\partial_a + b\partial_b + 2)[1, a, b] \log \\
&= \frac{1}{2}(a\partial_a + b\partial_b + 3)H_{2,1,1}^{CM}(a, b).
\end{aligned}$$

Similarly,

$$\begin{aligned}
H_{2,2,1}^{CM}(a, b) &= H_{1,1,0}^{(2)}(a, b) = -\partial_a H_{1,0,0}^{(2)}(a, b) \\
&= -\partial_a H_{2,1,1}^{CM}(a, b).
\end{aligned}$$

**5.4. Conclusion.** The possibilities to produce such formulas are endless. All these formulas can be obtained, of course, by performing partial fraction decompositions on the integrand of Eq. (4.1) resp. Eq. (4.2). However, the calculus of finite differences with its various rules provides a convenient framework which allows to obtain the formulas in a mechanical way.

### A. Divided differences

Divided differences have their origin in interpolation theory; they can be traced back to Newton. Although being standard textbook material in numerical analysis, let us give a very quick summary here; for a recent survey see [6], a classical reference is [14]. In the sequel all functions are assumed to be smooth.

**A.1.** Let  $f$  be a smooth function on a real interval  $I$  and let  $x_0, x_1, \dots$  a priori distinct points in  $I$ . Then one defines recursively the *divided differences*

$$\begin{aligned} [x_0]f &:= f(x_0), \\ [x_0, \dots, x_n]f &:= \frac{1}{x_0 - x_n} ([x_0, \dots, x_{n-1}]f - [x_1, \dots, x_n]f). \end{aligned} \quad (\text{A.1})$$

The first few divided differences are therefore

$$\begin{aligned} [x_0, x_1]f &= \frac{f(x_0)}{(x_0 - x_1)} + \frac{f(x_1)}{(x_1 - x_0)}, \\ [x_0, x_1, x_2]f &= \frac{f(x_0)}{(x_0 - x_1)(x_0 - x_2)} + \frac{f(x_1)}{(x_1 - x_0)(x_1 - x_2)} + \frac{f(x_2)}{(x_2 - x_0)(x_2 - x_1)}, \end{aligned}$$

and by induction one shows the explicit formula

$$[x_0, \dots, x_n]f = \sum_{k=0}^n f(x_k) \cdot \prod_{j=0, j \neq k}^n (x_k - x_j)^{-1}, \quad (\text{A.2})$$

resp. the Genocchi–Hermite integral formula [14, Sec. 1.6], [6, Sec. 9]<sup>5</sup>

$$\begin{aligned} [x_0, \dots, x_n]f &= \int_{\sum_{j=0}^n s_j = 1, s_j > 0}^n f^{(n)}\left(\sum_{j=0}^n s_j x_j\right) ds_1 \dots ds_n \\ &= \int_{0 \leq t_n \leq \dots \leq t_1 \leq 1} f^{(n)}\left((1 - t_1)x_0 + \dots + (t_{n-1} - t_n)x_{n-1} + t_n x_n\right) dt_1 \dots dt_n. \end{aligned} \quad (\text{A.3})$$

If  $f$  is even analytic, e.g. if  $f$  is already an interpolation polynomial, and if  $\gamma$  is a closed curve in the domain of  $f$  encircling the points  $x_0, \dots, x_n$  exactly once then by the Residue Theorem and Eq. (A.2) we have [14, Sec. 1.7]

$$[x_0, \dots, x_n]f = \frac{1}{2\pi i} \oint_{\gamma} f(\zeta) \prod_{j=0}^n (\zeta - x_j)^{-1} d\zeta. \quad (\text{A.4})$$

<sup>5</sup>According to the historical remarks in [6, Sec. 9] the formula is due to Genocchi who communicated it to Hermite in a letter.

**A.2. The confluent case.** From the right hand sides of Eq. (A.3) and Eq. (A.4) we see that  $[x_0, \dots, x_n]f$  is a smooth (analytic) function of the variables  $x_0, \dots, x_n$ . Therefore, one uses these formulas to extend the divided differences to the confluent case of repeated arguments. Thus, for any  $x_0, \dots, x_n \in I$ , regardless of being pairwise distinct or not,  $[x_0, \dots, x_n]f$  is a smooth (analytic) symmetric function of its arguments.

The divided differences can be calculated quite efficiently from the recursion system Eq. (A.1) and with some care this can also be extended to the confluent case [14, 1.8]. Alternatively, there is a differentiation formula relating a divided difference with repeated arguments to one with distinct arguments. This is obtained by differentiating by the parameters under the integral in Eq. (A.4) or in Genocchi–Hermite’s formula Eq. (A.3).

To explain this consider a multiindex  $\alpha = (\alpha_0, \dots, \alpha_n) \in \mathbb{N}^n$  and  $x_0, \dots, x_n \in I$ . We write  $[x_0^{\alpha_0+1}, \dots, x_n^{\alpha_n+1}]f$  for the divided difference  $[u_0, \dots, u_{|\alpha|+n}]f$  where the tuple  $(u_0, \dots, u_{|\alpha|+n})$  contains exactly  $\alpha_0 + 1$  copies of  $x_0$ ,  $\alpha_1 + 1$  copies of  $x_1$  etc. From Eq. (A.4) we infer [14, Sec. 1.8]

$$\begin{aligned} [x_0^{\alpha_0+1}, \dots, x_n^{\alpha_n+1}]f &= \frac{1}{2\pi i} \oint_{\gamma} f(\zeta) \prod_{j=0}^n (\zeta - x_j)^{-\alpha_j-1} d\zeta \\ &= \frac{1}{\alpha!} \partial_x^\alpha [x_0, \dots, x_n]f \\ &= \sum_{k=0}^n \frac{1}{\alpha_k!} \partial_{x_k}^{\alpha_k} \left( f(x_k) \prod_{j=0, j \neq k}^n (x_k - x_j)^{-\alpha_j-1} \right). \end{aligned} \quad (\text{A.5})$$

Recall that we are using the multiindex notation for partial derivatives and factorials, cf. Sec. 2.1.

**A.3. Leibniz rule.** The Leibniz rule for the divided difference of a product [6, Sec. 4]

$$[x_0, \dots, x_n](f \cdot g) = \sum_{j=0}^n [x_0, \dots, x_j]f \cdot [x_j, \dots, x_n]g, \quad (\text{A.6})$$

can be used to deduce interesting recursion formulas. Namely, taking  $g = \text{id}$  or  $\text{id}^2$  we find

$$\begin{aligned} [x_0, \dots, x_n](\text{id} f) &= x_0 \cdot [x_0, \dots, x_n]f + [x_1, \dots, x_n]f, \\ [x_0, \dots, x_n](\text{id}^2 f) &= x_0^2 \cdot [x_0, \dots, x_n]f \\ &\quad + (x_0 + x_1) \cdot [x_1, \dots, x_n]f + [x_2, \dots, x_n]f. \end{aligned}$$

Of course, this can be extended to arbitrary powers, cf. [14, Sec. 1.31].

**A.4. Substitution rule.** The following generalization of the recursion scheme Eq. (A.1) can be proved easily by induction (cf. [10, Prop. 11]). Given  $y_0, \dots, y_p$  put  $g(x) := [y_0, \dots, y_p, x]f$ . Then

$$[x_0, \dots, x_q]g = [y_0, \dots, y_p, x_0, \dots, x_q]f. \quad (\text{A.7})$$

## B. Homogeneous functions and totally characteristic differential operators

We muse a little about the totally characteristic derivative  $x\partial_x$ , certainly a little more than is barely necessary to see the formulas Eq. (4.6) and Eq. (4.7).

**B.1.** We will make frequent use of the *rising* and *falling* factorials (aka Pochhammer symbol) for which we adopt D. Knuth's notation [11, p. 50]<sup>6</sup>

$$(a)^{\bar{n}} := a \cdot (a+1) \cdot \dots \cdot (a+n-1), \quad (a)^{\bar{0}} := 1, \quad (\text{B.1})$$

$$(a)^{\underline{n}} := a \cdot (a-1) \cdot \dots \cdot (a-n+1), \quad (a)^{\underline{0}} := 1. \quad (\text{B.2})$$

Furthermore we denote by  $D_x = x\partial_x$  the totally characteristic derivative with respect to the variable  $x$ . For a polynomial  $p \in \mathbb{C}[t]$  we write  $p(\partial_x)$  resp.  $p(D_x)$  for  $\partial_x$  resp.  $D_x$  inserted into the indeterminate  $t$ . In particular, e.g.  $(D_x + k)^{\bar{n}}$  stands for  $D_x$  inserted into the polynomial  $(t+k)^{\bar{n}} \in \mathbb{C}[t]$ .

As an example we note the formula

$$\begin{aligned} x^a \partial_x^n x^b \partial_x^m (x^c \cdot) &= x^{a+b+c-n-m} \cdot (D_x + b + c - m)^{\underline{n}} \cdot (D_x + c)^{\bar{m}} \\ &= x^{a+b-n} \partial_x^m x^{n+m-b} \partial_x^n (x^{b+c-m} \cdot), \quad n, m \in \mathbb{N}, a, b, c \in \mathbb{C}. \end{aligned} \quad (\text{B.3})$$

This can be seen in a lot of ways. The obvious way is to expand the l. h. s. via the Leibniz' rule and then apply the Binomial Theorem. A much quicker way is to note that we have  $D_x x^z = z \cdot x^z$  for any complex number  $z$  and that for any such  $z$

$$\begin{aligned} x^a \partial_x^n x^b \partial_x^m x^{c+z} &= (z + b + c - m)^{\underline{n}} \cdot (z + c)^{\bar{m}} \cdot x^{z+a+b+c-n-m} \\ &= x^{a+b-n} \partial_x^m x^{n+m-b} \partial_x^n x^{b+c-m+z}, \end{aligned}$$

and since the l. h. s. and the r. h. s. of Eq. (B.3) are polynomials in  $D_x$ , they must be equal. Eq. (B.3) contains Eq. (5.12) as special case.

An immediate consequence of Eq. (B.3) is the fact that the family of differential operators  $x^{n-k} \partial_x^n (x^k \cdot)$ ,  $k, n \in \mathbb{Z}$ ,  $0 \leq k \leq n$ , is commuting.

We mention another important property of totally characteristic operators which is useful if one deals with the first integrand Eq. (4.1) which is a function of  $s_j x$ . Namely, if  $p(t) \in \mathbb{C}[t]$  is a complex polynomial and  $f$  a differentiable function then

$$p(D_x)f(xs) = p(D_s)f(xs) = (p(D)f)(xs). \quad (\text{B.4})$$

<sup>6</sup>He actually attributes it to A. Capelli (1893) and L. Toscano (1939).

**B.2. Homogeneous functions.** If  $\Gamma \subset \mathbb{R}^d$  is an open cone we denote by  $\mathcal{P}^a(\Gamma) = \mathcal{P}^a$  the space of smooth functions on  $\Gamma$  which are  $a$ -homogeneous, that is

$$f(\lambda \cdot \xi) = \lambda^a \cdot f(\xi).$$

Recall from Eq. (4.3) that the function  $M_\alpha^{(p)}(\cdot, z)$  is  $(-|\alpha| - p + z)$ -homogeneous.  $a$ -Homogeneous functions satisfy *Euler's identity*

$$\sum_{j=1}^q D_j f = a \cdot f. \tag{B.5}$$

Consequently, on  $\mathcal{P}^a$  we may replace  $D_1$  by  $-\sum_{j=2}^q D_j + a$ .

**B.3. The basic function  $b(x) = \frac{1}{1+x}$ .** Using the above mentioned rules the following formulas for the basic function  $b(x) = \frac{1}{1+x}$  occurring in the integral Eq. (4.1) can easily be derived<sup>7</sup>

$$\begin{aligned} \partial b^l &= -l \cdot b^{l+1}, \\ (D+l)b^l &= l \cdot b^{l+1}, \\ \partial^n b &= (-1)^n \cdot n! \cdot b^{n+1}, \\ (D+1)^{\bar{n}} b &= (D+n)^{\bar{n}} b = n! \cdot b^{n+1}, \\ x^{n-k} \partial^n x^k b(x) &= (D_x + k)^{\bar{n}} b(x) = (-1)^{n-k} \cdot n! \cdot x^{n-k} \cdot b(x)^{n+1}. \end{aligned} \tag{B.6}$$

**B.4. Proof of Eq. (4.6) and Eq. (4.7).** Recall from Eq. (4.3) that  $M_\alpha^{(p)}(\cdot, m)$  is  $(-|\alpha| - p + z)$ -homogeneous. Therefore, for  $\alpha = (\alpha_0, \alpha')$  we infer from Eq. (4.5) and Eq. (B.3) for  $m \in \{0, 1, \dots, |\alpha'| + p - 1\}$

$$\begin{aligned} s_0^{\alpha_0} M_\alpha^{(p)}(s, m) &= \frac{(-1)^{\alpha_0}}{\alpha_0!} s_0^{\alpha_0} \partial_{s_0}^{\alpha_0} M_{\alpha'}^{(p)}(s, m) \\ &= \frac{(-1)^{\alpha_0}}{\alpha_0!} (D_{s_0})^{\alpha_0} M_{\alpha'}^{(p)}(s, m), \end{aligned} \tag{B.7}$$

and since  $M_{\alpha'}^{(p)}(\cdot, m)$  is  $(-|\alpha'| - p + m)$ -homogeneous we may replace  $(D_{s_0})^{\alpha_0}$  by

$$\begin{aligned} \left(-\sum_{k=1}^p D_{s_j} - |\alpha'| - p + m\right)^{\alpha_0} &= (-1)^{\alpha_0} \left(\sum_{k=1}^p D_{s_j} + |\alpha'| + p - m\right)^{\bar{\alpha}_0} \\ &= (-1)^{\alpha_0} \left(\sum_{k=1}^p D_{s_j} + |\alpha| + p - 1 - m\right)^{\alpha_0}. \end{aligned} \tag{B.8}$$

From Eq. (B.7) and (B.8) the remaining claims of Proposition 4.1 follow. □

<sup>7</sup>Of course, they can also be derived by brute force.

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