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Local invariants of conformally deformed non-commutative tori II: Multiple operator integrals

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A B S T R A C T

We explicitly compute the local invariants (heat kernel coefficients) of a conformally deformed non-commutative d-torus using multiple operator integrals. We derive a recursive formula that easily produces an explicit expression for the local invariants of any order k and in any dimension d. Our recursive formula can conveniently produce all formulas related to the modular operator, which before were obtained in incremental steps for $d \in \{2, 3, 4\}$ and $k \in \{0, 2, 4\}$. We exemplify this by writing down some known ($k = 2$, $d = 2$) and some novel ($k = 2$, $d \geq 3$) formulas in the modular operator.

1. Introduction

Studying the heat trace expansion on a non-commutative manifold, and computing the respective local invariants (i.e., the non-commutative heat kernel coefficients), is vital for two reasons. Firstly, the heat kernel coefficients play a major role in quantum field theory (cf. [44]), and if space turns out to be non-commutative at small scale, these coefficients

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will need to be generalised. Secondly, the local invariants allow to extract geometric information from the spectrum of a Laplace-type operator, and they are therefore good starting points to extend geometric concepts to the setting of non-commutative geometry.

We shall focus on the non-commutative d-tori $\mathbb{T}^d_\theta$, as they are prime examples of non-commutative spaces. A benefit of these examples is that they have clear-cut non-commutative analogues $C^\infty(\mathbb{T}^d_\theta)$ and $L_\infty(\mathbb{T}^d_\theta)$ of the commutative algebras $C^\infty(\mathbb{T}^d)$ and $L_\infty(\mathbb{T}^d)$, together with a faithful representation λ_l on the Hilbert space $L_2(\mathbb{T}^d_\theta)$, which is an analogue of $L_2(\mathbb{T}^d)$, and a trace $\tau : L_\infty(\mathbb{T}^d_\theta) \to \mathbb{C}$, which is an analogue of integration; see the definitions in Section 2.2.

The local invariants $I_k(P)$ of an operator P acting in $L_2(\mathbb{T}^d_\theta)$ are the unique coefficients occurring in the heat trace expansion, which is the asymptotic expansion

$$\mathrm{Tr}(\lambda_l(y)e^{-tP}) \sim \sum_{\substack{k\geq 0\\ k=0 \bmod 2}} t^{\frac{k-d}{2}}\tau(y\, I_k(P)), \quad t\downarrow 0 \qquad (y\in L_\infty(\mathbb{T}^d_\theta)). \tag{1.1}$$

In [43] it was shown that this expansion exists if (and in particular e^{-tP} is trace class if) P is self-adjoint and of the form

$$P = \lambda_l(x)\Delta + \sum_{i=1}^d \lambda_l(a_i)D_i + \lambda_l(a) \quad \text{for some} \quad x, a_i, a \in C^\infty(\mathbb{T}^d_\theta), \tag{1.2}$$

with x positive and invertible. Here, $\Delta = \sum_{i=1}^d D_i^2$ and D_i is the i^{th} directional derivative which, again, is defined in Section 2.2. In this generalised sense, P is a strongly elliptic differential operator. Besides the existence of the asymptotic expansion, [43] shows that $I_k(P) \in C^\infty(\mathbb{T}^d_\theta)$, so $y \mapsto \tau(y\, I_k(P))$ can informally be thought of as 'integration' against a smooth 'function' $I_k(P)$. The goal of this paper is to explicitly compute $I_k(P)$ for this class of P (those of the form (1.2) with x positive and invertible).

One motivation to consider this class of P is the vibrant research program that surrounds the local invariants of the so-called conformally deformed non-commutative torus, a research program that was initiated by the papers [4,7,8]. The classical limit of the non-commutative torus is simply the flat torus $\mathbb{T}^d$, which holds no interesting geometry, and likewise $I_k(\Delta)$ is trivial. Geometric non-triviality is added to the torus in [4] by an adjustment analogous to a conformal scaling of the metric, and the result is called the conformally deformed non-commutative torus. For our purposes, we can capture this conformal scaling (see, e.g., [7]) by replacing the Laplacian by operators P of the form (1.2) and keeping the same Hilbert space, algebra, and representation.

A main goal in the research program mentioned above is to express the local invariants $I_k(P)$ as closed formulas involving functional calculus applied to the modular operator defining the conformal scaling, as done in [7,13] for $k = 2$, $d = 2$.

New functions acting by this 'modular functional calculus' were found for $d = 4, k = 2$ in [14], for $d = 2, k = 4$ in [6], for $d = 3, k = 4$ in [11], and for $d \geq 2, k = 2$ in [17], and to understand and sometimes simplify the vast calculations in these papers, significant progress has been made in [12,28–30,32]. In this context, various geometric notions were lifted to the non-commutative setting in [8,9,13,15,21–23,31,34,37,40,45] *et cetera*, giving further foundation and motivation for the calculation of the local invariants in terms of modular functional calculus, but not yet extending that calculation to higher dimension and higher order. In most of the papers mentioned above, the local invariants are obtained by means of the zeta function associated with P.

Seemingly, these results are completely distinct from the geometric formulas (found, e.g., in [18]) for the local invariants in the commutative case – the heat kernel coefficients. These coefficients, also called Gilkey–Seeley–DeWitt coefficients, are extremely useful in quantum field theory and other parts of physics (cf. [44]) and their extensions to non-commutative manifolds are likely essential to any new quantum theory of particles or gravity. For example, the confrontation of the spectral standard model [3] with particle physics, which so far looks promising (cf. [2]), relies precisely on this heat trace expansion for bundles over manifolds (cf. [42]), while in non-commutative quantum field theories like [19] the underlying space itself is non-commutative, and bares resemblance to a non-commutative torus (cf. [39]). Similarly, the non-commutative d-torus arises from matrix theory compactification, as explained in [5,27].

The above shows why it is notable that, in [24–26], geometric formulas for the heat kernel coefficients were derived in an operator-algebraic way (by means of a Volterra series), although the fully non-commutative torus was not yet tackled.

In this paper, we give a way to compute $I_k(P)$ explicitly for every $d \in \mathbb{N}_{\geq 2}$ and every $k \in \mathbb{Z}_{\geq 0}$, by making use of the full power of multiple operator integration theory, and using the description of $I_k(P)$ that in [43] led to the existence of the asymptotic expansion (1.1) for P of the form (1.2). Instead of the abstract modular functional calculus employed by Connes and others, we use the framework of multiple operator integrals (a short introduction for the non-affiliate is given in Section 2.1), and we show how the two approaches are related. We also relate our approach to the (almost) commutative approach of [24–26], which (as argued in the two paragraphs above) opens up a realm of potential applications in physics.

Our main result is a compact expression for $I_k(P)$ that involves a simple recursive rule. When a specific k is chosen, this expression can be recursively expanded, and the resulting expressing for $I_k(P)$ is a sum of explicit multiple operator integrals (that in many cases can be computed algebraically, as in Remark 2.2). The amount of terms blows up rapidly (1 term for $k = 0$, 13 terms for $k = 2$, 1046 terms for $k = 4$, 140845 terms for $k = 6$, *et cetera*).

Furthermore, we show how one can straightforwardly obtain all functions acting by modular functional calculus from the just-mentioned expressions in terms of multiple operator integrals. Thus we conclude a list [6,7,17,13,14,11] of advancements in which such functions were found for slowly increasing k and d. Our approach yields a substantial insight into the structure and appearance of such functions in [6,7,17,13,14,11], namely, as the results of a recursive procedure that starts with a simple expression, and increasingly jumbles up the result in each step. In particular, our recursive structure explains the appearance of divided differences in these functions as a result of a commutator rule for multiple operator integrals that is also central to [35], and hence (through the arguments of [28,33]) sheds light on the functional relations of [6,7].

Passing from multiple operator integrals to modular functional calculus is quite simple, which we exemplify by producing some known and some novel modular formulas.

Finally, we hope the novel expression for $I_k(P)$ in our main result inspires generalisation to more general elliptic operators, including the settings of [10,24,31] *et cetera*.

This paper is structured as follows. After introducing the beautiful subject of multiple operator integration and fixing our notation in Section 2, we give a comprehensive summary of our main results and applications in Section 3. Section 4 contains some groundwork. After that, the proof of our main theorem, Theorem 3.3, will span the whole of Sections 5, 6, and 7. In Section 8 we apply our main result to the case $k = 2$ and prove Corollary 3.6 and Theorem 3.8. The connection with modular functional calculus is made in Section 9, and the connection with the commutative case is made in Section 10. Appendix A comments on the accompanying python program.

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2. Preliminaries

We let $\mathbb{N} = \{1, 2, \ldots\}$, $\mathbb{Z}_+ = \mathbb{Z}_{\geq 0}$, $\mathbb{T} := \mathbb{R}/\mathbb{Z}$, $\mathbb{R}_- = (-\infty, 0)$. On a suitable set X we let $C^\infty(X), L_1(X), L_2(X)$ denote the smooth, Lebesgue integrable, and square-integrable functions, respectively. For $n \in \mathbb{Z}^m$ we write $|n|_1 := \sum_{i=1}^m |n_i|$. The bounded operators on a Hilbert space $\mathcal{H}$ are denoted $\mathcal{B}(\mathcal{H})$.

2.1. Multiple operator integrals

2.1.1. Introduction

The role that multiple operator integrals play for local invariants has never been clearly spelled out (and was but mentioned in [33]). However, when computing local invariants, one frequently (e.g. in [13,24–26,28,32]) encounters integrals that look roughly similar to, for example,

$$\int_0^1 \int_0^{s_1} e^{(s_1-1)x} V_1 \, e^{(s_2-s_1)x} V_2 \, e^{-s_2 x} \, ds_2 \, ds_1; \tag{2.1}$$

$$\int_{\mathbb{R}} \frac{1}{x+i\lambda} V_1 \frac{1}{x+i\lambda} V_2 \frac{1}{x+i\lambda} \frac{e^{i\lambda}}{2\pi} \, d\lambda; \tag{2.2}$$

or any other integral over an alternating product of bounded operators V_1, V_2 and functions of a self-adjoint operator x. These are in fact special cases of multiple operator integrals, namely, integrals of the form (2.4) in the following definition.

Definition 2.1. Let $n \in \mathbb{N}$, and let x be a (possibly unbounded) self-adjoint operator in a separable Hilbert space $\mathcal{H}$, with spectrum $\operatorname{spec}(x)$. Let $\phi : \operatorname{spec}(x)^{n+1} \to \mathbb{C}$ be given by

$$\phi(\alpha_0, \dots, \alpha_n) = \int_\Omega a_0(\alpha_0, \lambda) a_1(\alpha_1, \lambda) \cdots a_n(\alpha_n, \lambda)\, d\lambda, \tag{2.3}$$

for bounded measurable functions $a_0, \dots, a_n : \operatorname{spec}(x) \times \Omega \to \mathbb{C}$ and a finite measure space (Ω, λ). The multiple operator integral is the multilinear function $T_\phi^x : \mathcal{B}(\mathcal{H})^{\times n} \to \mathcal{B}(\mathcal{H})$ defined by

$$T_\phi^x(V_1, \dots, V_n)\psi := \int_\Omega a_0(x, \lambda) V_1 a_1(x, \lambda) \cdots V_n a_n(x, \lambda) \psi \, d\lambda, \tag{2.4}$$

for $V_1, \dots, V_n \in \mathcal{B}(\mathcal{H})$, $\psi \in \mathcal{H}$.

This definition was given in [1, Definition 4.1] and [36], and it is a simple but crucial result of [1, Lemma 4.3] and [36, Lemma 3.1] that T_ϕ^x only depends on the function ϕ, but not on the particular choice of the functions $a_0, \dots, a_n$ in the representation (2.3), as the notation suggests. For example, under reasonable assumptions, (2.1) equals (2.2).[1] This explains why the literature sometimes contains different procedures to calculate the same thing. Providing an elegant unified picture is not the only purpose of multiple operator integration (and we ensure the critical reader that we are not merely casting known results into new notation). The theory of multiple operator integration provides extremely strong results on the analytical properties of integrals like (2.1) and (2.2), and moreover, the formalism often leads to completely new results or extensive generalisations of known ones. (See [41] for an overview of theory and applications.)

2.1.2. Basic results on multiple operator integrals

If $n = 0$, then Definition 2.1 recovers functional calculus:

$$T_\phi^x() = \phi(x).$$

Moreover, if $V_1, \dots, V_n$ commute with x then $T_\phi^x(V_1, \dots, V_n)$ by definition reduces to $\phi(x, \dots, x) V_1 \cdots V_n$. This paper deals exclusively with bounded $x \in \mathcal{B}(\mathcal{H})$, so let us assume this from now on.

[1] To see this, one takes x positive and invertible, replaces e^{sx} and $\frac{1}{x+i\lambda}$ by bounded functions of x, and works out the second divided difference (definition below) of $x \mapsto e^{-x}$ in two ways. By the well-definedness of the multiple operator integral, the equality of functions implies an equality of operators.

The function ϕ is called the symbol of T^x_ϕ, and it is often defined on a region strictly surrounding $\mathrm{spec}(x)^{n+1}$ (such as $\mathbb{R}^{n+1}$), in which situation we write $T^x_\phi = T^x_{\phi_{|\mathrm{spec}(x)^{n+1}}}$ as one would expect. The symbols we encounter most are *divided differences* $\phi = f^{[n]} \in C(\mathbb{R}^{n+1})$ of some $f \in C^n(\mathbb{R})$, defined recursively by

$$f^{[0]}(\alpha_0) := f(\alpha_0); \tag{2.5}$$

$$f^{[n]}(\alpha_0, \dots, \alpha_n) := \frac{f^{[n-1]}(\alpha_0, \alpha_1, \dots, \alpha_{n-1}) - f^{[n-1]}(\alpha_1, \dots, \alpha_n)}{\alpha_0 - \alpha_n}, \tag{2.6}$$

for $\alpha_0 \neq \alpha_n$, and extended continuously to $\alpha_0 = \alpha_n$. It is well-known that $f^{[n]}$ is symmetric in its arguments and satisfies $f^{[n]}(\alpha, \dots, \alpha) = \frac{1}{n!} f^{(n)}(\alpha)$. Moreover, if $\widehat{f^{(n)}} \in L_1(\mathbb{R})$, then we have

$$f^{[n]}(\alpha_0, \dots, \alpha_n) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_{S^n} \widehat{f^{(n)}}(t) e^{it\lambda_0\alpha_0} \cdots e^{it\lambda_n\alpha_n} \, d\lambda \, dt, \tag{2.7}$$

where λ is the flat measure on the simplex $S^n = \{\lambda \in \mathbb{R}^{n+1}_{\geq 0} : \sum_{j=0}^n \lambda_j = 1\}$ with $\lambda(S^n) = 1/n!$. By comparing (2.7) to (2.3), we notice that $T^x_{f^{[n]}}$ is defined whenever $f \in C^n(\mathbb{R})$ and $\widehat{f^{(n)}} \in L_1(\mathbb{R})$. Let $I \subseteq \mathbb{R}$ be a bounded neighbourhood of $\mathrm{spec}(x)$. By (2.5) and (2.6), $f \mapsto T^x_{f^{[n]}}$ factors through $f \mapsto f|_I$. Moreover, any $f \in C^\infty(I)$ can be extended to a Schwartz function on $\mathbb{R}$, which satisfies (2.7). Therefore, $T^x_{f^{[n]}}$ is defined for any $f \in C^\infty(I)$. Some important identities in this case are (cf. [35, Lemma 14])

$$\begin{aligned}
&T^x_{f^{[n]}}(V_1, \dots, V_j, yV_{j+1}, \dots, V_n) - T^x_{f^{[n]}}(V_1, \dots, V_j y, V_{j+1}, \dots, V_n) \\
&= T^x_{f^{[n+1]}}(V_1, \dots, V_j, [x,y], V_{j+1}, \dots, V_n); \\
&T^x_{f^{[n]}}(yV_1, \dots, V_n) - yT^x_{f^{[n]}}(V_1, \dots, V_n) = T^x_{f^{[n+1]}}([x,y], V_1, \dots, V_n); \\
&T^x_{f^{[n]}}(V_1, \dots, V_n)y - T^x_{f^{[n]}}(V_1, \dots, V_n y) = T^x_{f^{[n+1]}}(V_1, \dots, V_n, [x,y]); \\
&f(x)y - yf(x) = T^x_{f^{[0]}}()y - yT^x_{f^{[0]}}() = T^x_{f^{[1]}}([x,y]),
\end{aligned} \tag{2.8}$$

for $x, y, V_j \in \mathcal{B}(\mathcal{H})$. In this paper we often see $f = F_{k,d}$, where $F_{k,d}$ is our notation for the $\frac{k}{2}^{\text{th}}$ order primitive of $\alpha \mapsto \alpha^{-\frac{d}{2}}$ on $I = (0, \|x\|+1)$, which is a bounded neighbourhood of $\mathrm{spec}(x)$ when x is a positive invertible bounded operator. In the literature, the dimension d of the (non-commutative) space is often even and the order k (appearing in $I_k(P)$) is often small. In these abundant cases the multiple operator integral is extremely explicit:

Remark 2.2. Suppose that d is even and that $k < d$. Then $F_{k,d}$ is an integer power function, so for every $n \in \mathbb{N}$ there exists a finite $L \subseteq \mathbb{Z}^{n+1}$ and some constants c_l such that, for all $\alpha_j > 0$,

$$F^{[n]}_{k,d}(\alpha_0, \dots, \alpha_n) = \sum_{l \in L} c_l \alpha_0^{l_0} \cdots \alpha_n^{l_n}.$$

As a consequence, the multiple operator integral is a purely algebraic expression,

$$T^{x}_{F^{[n]}_{k,d}}(V_1,\dots,V_n)=\sum_{l\in L}c_l x^{l_0}V_1x^{l_1}\cdots V_nx^{l_n},$$

for all $V_j\in\mathcal{B}(\mathcal{H})$ and positive invertible $x\in\mathcal{B}(\mathcal{H})$.

2.2. Non-commutative torus

Regarding the non-commutative torus, we use the definitions of [43], which we only briefly recall in this section. We omit the proofs of the folklore assertions below, some of which can be found in [43, §2].

For any $d\in\mathbb{N}_{\geq 2}$, we let $\theta\in M_d(\mathbb{R}^d)$ be an antisymmetric matrix. Let A_θ be the unital *-algebra generated by formal symbols $U_1,\dots,U_d$ satisfying $U_k^*U_k=U_kU_k^*=1$ and $U_kU_l=e^{2\pi i\theta_{kl}}U_lU_k$, and write $U^n:=U_1^{n_1}\cdots U_d^{n_d}$ for all $n\in\mathbb{Z}^d$. We define a linear function $\tau:A_\theta\to\mathbb{C}$ by $\tau(\sum_n c_nU^n):=c_0$. We let $L_2(\mathbb{T}^d_\theta)$ be the completion of A_θ in the norm $\|a\|:=\langle a,a\rangle^{\frac12}$ defined by the (nondegenerate) inner product $\langle a,b\rangle:=\tau(a^*b)$, which makes $\mathcal{H}:=L_2(\mathbb{T}^d_\theta)$ a separable Hilbert space. We define $D_k(\sum_n c_nU^n):=\sum_n c_nn_kU^n$ on A_θ, and let $C^\infty(\mathbb{T}^d_\theta)$ be the completion of A_θ in the (Fréchet) seminorms $a\mapsto\|D^\alpha a\|$, $\alpha\in\mathbb{Z}^d_+$, where $D^\alpha:=D_1^{\alpha_1}\cdots D_d^{\alpha_d}$. Each D^α extends to a self-adjoint operator densely defined in $L_2(\mathbb{T}^d_\theta)$, with $C^\infty(\mathbb{T}^d_\theta)=\cap_\alpha\operatorname{dom}D^\alpha$. Hence, $C^\infty(\mathbb{T}^d_\theta)$ is stable under holomorphic functional calculus. We represent A_θ on $L_2(\mathbb{T}^d_\theta)$ by $\lambda_l(a)b:=ab$, and denote by $L_\infty(\mathbb{T}^d_\theta)$ the corresponding weak closure of A_θ, a von Neumann algebra with operator norm denoted $\|\cdot\|_\infty$. We identify $C^\infty(\mathbb{T}^d_\theta)\subseteq L_\infty(\mathbb{T}^d_\theta)$ and $L_2(\mathbb{T}^d_\theta)\subseteq L_\infty(\mathbb{T}^d_\theta)$. Both τ and λ_l extend continuously to $L_\infty(\mathbb{T}^d_\theta)$, giving a faithful tracial state $\tau:L_\infty(\mathbb{T}^d_\theta)\to\mathbb{C}$ and a faithful representation (injective *-homomorphism) $\lambda_l:L_\infty(\mathbb{T}^d_\theta)\to\mathcal{B}(L_2(\mathbb{T}^d_\theta))$.

3. Summary of main results

Before coming to our main result, it is important to get well acquainted with the recursive structure that lies at its core.

3.1. Recursive structure

We let $\mathbf{D}_1,\dots,\mathbf{D}_d$ be the formal symbols of the polynomial algebra $\mathbb{C}[\mathbf{D}_1,\dots,\mathbf{D}_d]$, i.e., we impose only the relation $\mathbf{D}_i\mathbf{D}_j=\mathbf{D}_j\mathbf{D}_i$ for all $i,j\in\{1,\dots,d\}$. We write $\mathbf{D}^\alpha:=\mathbf{D}_1^{\alpha_1}\cdots\mathbf{D}_d^{\alpha_d}$ for all $\alpha\in\mathbb{Z}^d_+$. We then define the free left $C^\infty(\mathbb{T}^d_\theta)$-module

$$\mathcal{X}:=\operatorname{span}\big\{b\mathbf{D}^\alpha:\ b\in C^\infty(\mathbb{T}^d_\theta),\alpha\in\mathbb{Z}^d_+\big\},$$

generated by the set of formal symbols $\{\mathbf{D}^\alpha:\ \alpha\in\mathbb{Z}^d_+\}$. In other words, $\mathcal{X}$ is the d-variable polynomial algebra with scalars in $C^\infty(\mathbb{T}^d_\theta)$. We identify $C^\infty(\mathbb{T}^d_\theta)\subseteq\mathcal{X}$ as the subset of constant polynomials, i.e., we abbreviate $b\mathbf{D}^0$ by b for all $b \in C^\infty(\mathbb{T}^d_\theta)$. We also briefly write $D_i x = D_i(x) \in C^\infty(\mathbb{T}^d_\theta)$.

Definition 3.1. Let $x \in C^\infty(\mathbb{T}^d_\theta)$ be self-adjoint and $f : \mathbb{R} \to \mathbb{R}$ be smooth when restricted to the spectrum of x. For every $m \in \mathbb{Z}_+$, we recursively define multilinear mappings $\mathbf{T}^{x,m}_f : \mathcal{X}^{\times m} \to C^\infty(\mathbb{T}^d_\theta)$ by firstly setting

$$\mathbf{T}^{x,m}_f(b_1, \dots, b_m) := T^x_{f^{[m]}}(b_1, \dots, b_m),$$

for all $b_1, \dots, b_m \in C^\infty(\mathbb{T}^d_\theta) \subseteq \mathcal{X}$, secondly setting

$$\begin{aligned}\mathbf{T}^{x,m}_f(\mathbf{B}_1, \dots, \mathbf{B}_{k-1}, \mathbf{B}_k\mathbf{D}_i, b_{k+1}, \dots, b_m)&\\ := \mathbf{T}^{x,m+1}_f(\mathbf{B}_1, \dots, \mathbf{B}_k, D_i x, b_{k+1}, \dots, b_m)&\\ + \mathbf{T}^{x,m}_f(\mathbf{B}_1, \dots, \mathbf{B}_k, D_i b_{k+1}, b_{k+2}, \dots, b_m)&\\ + \mathbf{T}^{x,m}_f(\mathbf{B}_1, \dots, \mathbf{B}_k, b_{k+1}\mathbf{D}_i, b_{k+2}, \dots, b_m),& \qquad (3.1)\end{aligned}$$

for all $\mathbf{B}_1, \dots, \mathbf{B}_m \in \mathcal{X}$ and $k < m$, and lastly setting

$$\mathbf{T}^{x,m}_f(\mathbf{B}_1, \dots, \mathbf{B}_{m-1}, \mathbf{B}_m\mathbf{D}_i) := \mathbf{T}^{x,m+1}_f(\mathbf{B}_1, \dots, \mathbf{B}_m, D_i x). \qquad (3.2)$$

Well-definedness of $\mathbf{T}^{x,m}_f$ is shown in Lemma 4.1.

Example 3.2. As a simple example of Definition 3.1 we have

$$\begin{aligned}\mathbf{T}^{x,2}_f(a, b\mathbf{D}_i) &= \mathbf{T}^{x,3}_f(a, b, D_i x)\\ &= T^x_{f^{[3]}}(a, b, D_i x). \qquad (3.3)\end{aligned}$$

A similar example is

$$\begin{aligned}\mathbf{T}^{x,2}_f(a, b\mathbf{D}_i\mathbf{D}_j) =& \mathbf{T}^{x,3}_f(a, b\mathbf{D}_i, D_j x)\\ =& \mathbf{T}^{x,4}_f(a, b, D_i x, D_j x) + \mathbf{T}^{x,3}_f(a, b, D_i D_j x) + \mathbf{T}^{x,3}_f(a, b, D_j x\mathbf{D}_i)\\ =& T^x_{f^{[4]}}(a, b, D_i x, D_j x) + T^x_{f^{[3]}}(a, b, D_i D_j x) + T^x_{f^{[4]}}(a, b, D_j x, D_i x).\end{aligned}$$

Another instructive example is

$$\begin{aligned}\mathbf{T}^{x,3}_f(a\mathbf{D}_i, b, c) =& T^x_{f^{[4]}}(a, D_i x, b, c) + T^x_{f^{[3]}}(a, D_i b, c) + \mathbf{T}^{x,3}_f(a, b\mathbf{D}_i, c)\\ =& T^x_{f^{[4]}}(a, D_i x, b, c) + T^x_{f^{[3]}}(a, D_i b, c) + T^x_{f^{[4]}}(a, b, D_i x, c)\\ &+ T^x_{f^{[3]}}(a, b, D_i c) + T^x_{f^{[4]}}(a, b, c, D_i x).\end{aligned}$$

An only slightly more involved expression like

$$\mathbf{T}_f^{x,3}(a\mathbf{D}_i\mathbf{D}_j, b\mathbf{D}_k, c)$$

already produces 145 terms (the reader is encouraged to check why), which can be straightforwardly obtained if one has enough time (or a computer at hand).

The above example illustrates that, however complicated $\mathbf{B}_1, \ldots, \mathbf{B}_m \in \mathcal{X}$ might be, $\mathbf{T}_f^{x,m}(\mathbf{B}_1, \ldots, \mathbf{B}_m)$ can always be written as a sum of multiple operator integrals with arguments in $C^\infty(\mathbb{T}_\theta^d)$. The above example also illustrates that, morally, we have

$$\mathbf{T}_f^{x,m}(b_1\mathbf{D}^{\alpha_1}, \ldots, b_m\mathbf{D}^{\alpha_m}) = \text{“}\, T_{f^{[m]}}^{\lambda_l(x)}(\lambda_l(b_1)D^{\alpha_1}, \ldots, \lambda_l(b_m)D^{\alpha_m})(1)\,\text{”}, \tag{3.4}$$

in the sense that, if we would take (2.8) at face value, we would have (using $D_i 1 = 0$)

$$\begin{aligned} \text{“}T_{f^{[2]}}^{\lambda_l(x)}(\lambda_l(a), \lambda_l(b)D_i)(1)\text{”} &= T_{f^{[3]}}^{\lambda_l(x)}(\lambda_l(a), \lambda_l(b), [D_i, \lambda_l(x)])(1) \\ &= T_{f^{[3]}}^{\lambda_l(x)}(\lambda_l(a), \lambda_l(b), \lambda_l(D_i x))(1) \\ &= T_{f^{[3]}}^{x}(a, b, D_i x), \end{aligned}$$

which mimics (3.3), and similarly for the other defining properties of $\mathbf{T}_f^{x,m}$. However, the unbounded arguments of the multiple operator integrals between quotes warrant some caution. The moral identity (3.4) is made rigorous by Corollary 7.1, which forms a crucial step towards our main theorem. A unifying interpretation has recently been put forth in [20].

The final ingredients for our main result are the elements that we use as inputs of the mappings $\mathbf{T}_f^{x,m}$. For every $x, a_1, \ldots, a_d, a \in C^\infty(\mathbb{T}_\theta^d)$, every $m \in \mathbb{N}$, every subset $\mathscr{A} \subseteq \{1, \ldots, m\}$, and every function $\iota : \mathscr{A} \to \{1, \ldots, d\}$, we define $\mathbf{W}_1^{\mathscr{A},\iota}, \ldots, \mathbf{W}_m^{\mathscr{A},\iota} \in \mathcal{X}$ by

$$\mathbf{W}_j^{\mathscr{A},\iota} = \begin{cases} \mathbf{A}_{\iota(j)} & (j \in \mathscr{A}); \\ \mathbf{P}, & (j \notin \mathscr{A}), \end{cases} \tag{3.5}$$

where (for all $i \in \{1, \ldots, d\}$)

$$\mathbf{A}_i := 2x\mathbf{D}_i + a_i, \quad \mathbf{P} := x\sum_{i=1}^d \mathbf{D}_i^2 + \sum_{i=1}^d a_i\mathbf{D}_i + a \quad \in \quad \mathcal{X}. \tag{3.6}$$

3.2. Main result

Our main result is formulated as follows.

Theorem 3.3. *Let $d \in \mathbb{N}_{\geq 2}$, $k \in 2\mathbb{Z}_+$, let $x, a_1, \ldots, a_d, a \in C^\infty(\mathbb{T}_\theta^d)$ be self-adjoint with x positive and invertible, and define P by (1.2). The k^{th} order local invariant of P occurring in the asymptotic expansion (1.1) takes the form*

$$I_k(P) = (-1)^{\frac{k}{2}} \pi^{\frac{d}{2}} \sum_{\frac{k}{2} \leq m \leq k} \sum_{\substack{\mathscr{A} \subseteq \{1,\dots,m\} \\ |\mathscr{A}|=2m-k}} \sum_{\iota : \mathscr{A} \to \{1,\dots,d\}} c_d^{(\iota)} \mathbf{T}^{x,m}_{F_{k,d}}(\mathbf{W}_1^{\mathscr{A},\iota}, \dots, \mathbf{W}_m^{\mathscr{A},\iota}), \quad (3.7)$$

where $F_{k,d}$ is any $\frac{k}{2}^{th}$ order primitive of $\alpha \mapsto \alpha^{-\frac{d}{2}}$ and

$$c_d^{(\iota)} := \frac{1}{\mathrm{vol}(\mathbb{S}^{d-1})} \int_{\mathbb{S}^{d-1}} \prod_{j \in \mathscr{A}} u_{\iota(j)} \, du.$$

For non-self-adjoint P the right-hand side of (3.7) still exists, and we may take this as the extended definition of $I_k(P)$ (as it coincides with Definition 4.6).

Remark 3.4. An explicit $\frac{k}{2}^{\text{th}}$ order primitive of $\alpha \mapsto \alpha^{-\frac{d}{2}}$ is given by

$$F_{k,d}(\alpha) := \begin{cases} (-1)^{\frac{k}{2}} \frac{\Gamma(\frac{d}{2} - \frac{k}{2})}{\Gamma(\frac{d}{2})} \alpha^{\frac{k-d}{2}} & \text{if } d \text{ is odd or } k < d; \\ (-1)^{\frac{d}{2}-1} \frac{1}{(\frac{d}{2}-1)!(\frac{k}{2}-\frac{d}{2})!} \alpha^{\frac{k-d}{2}} \log(\alpha) & \text{if } d \text{ is even and } k \geq d. \end{cases}$$

In particular, we have $F_{2,2} = \log$.

Remark 3.5. The constants $c_d^{(\iota)}$ are rational, invariant under permutations on the domain and range of ι, and, lastly, easy to compute. Writing $n_j := |\iota^{-1}(\{j\})|$, we have (cf. [16])

$$c_d^{(\iota)} = \begin{cases} \frac{(d-2)!! \prod_{j=1}^d (n_j - 1)!!}{(|n|_1 + d - 2)!!} & \text{if } n_1, \dots, n_d \text{ are even;} \\ 0 & \text{otherwise.} \end{cases}$$

Here we use the usual convention $(-1)!! = 1$.

To illustrate what (3.7) means in practice, we note that for $k = 0, 2, 4$ it states that (cf. Section 8)

$$\pi^{-\frac{d}{2}} I_0(P) = \mathbf{T}^{x,0}_{F_{0,d}}();$$

$$-\pi^{-\frac{d}{2}} I_2(P) = \mathbf{T}^{x,1}_{F_{2,d}}(\mathbf{P}) + \sum_{i=1}^d \frac{1}{d} \mathbf{T}^{x,2}_{F_{2,d}}(\mathbf{A}_i, \mathbf{A}_i);$$

$$\begin{aligned}\pi^{-\frac{d}{2}} I_4(P) = &\mathbf{T}^{x,2}_{F_{4,d}}(\mathbf{P}, \mathbf{P}) + \sum_{i=1}^d \frac{1}{d} \Big(\mathbf{T}^{x,3}_{F_{4,d}}(\mathbf{P}, \mathbf{A}_i, \mathbf{A}_i) + \mathbf{T}^{x,3}_{F_{4,d}}(\mathbf{A}_i, \mathbf{P}, \mathbf{A}_i) \\ &+ \mathbf{T}^{x,3}_{F_{4,d}}(\mathbf{A}_i, \mathbf{A}_i, \mathbf{P}) \Big) + \sum_{i,j,k,l=1}^d c_d^{(i,j,k,l)} \mathbf{T}^{x,4}_{F_{4,d}}(\mathbf{A}_i, \mathbf{A}_j, \mathbf{A}_k, \mathbf{A}_l),\end{aligned}$$

but the real beauty of (3.7) is that this compact expression holds for any k.

3.3. Consequences of our main result

Straightforward corollaries of Theorem 3.3 are obtained by fixing k and expanding the recursive definition of $\mathbf{T}_f^{x,m}$ (as in Remark 2.2) into explicit sums of multiple operator integrals with arguments in the non-commutative torus. The resulting formula for I_0 is nothing new, namely

$$\pi^{-\frac{d}{2}} I_0(P) = T^x_{F^{[0]}_{0,d}}() = F_{0,d}(x) = x^{-\frac{d}{2}}.$$

However, the resulting formula for the second order local invariant I_2, which is sometimes called the scalar curvature, is already of note. We obtain the following explicit expression, which for $d = 2, 4$ can be used to recover the results of [7,12–14] (more on this later).

Corollary 3.6. *For any dimension $d \in \mathbb{N}_{\geq 2}$, and P acting in $L_2(\mathbb{T}^d_\theta)$ of the form (1.2) for positive invertible x, the second order local invariant of P is computed by*

$$\begin{aligned}
-\pi^{-\frac{d}{2}} I_2(P) = &\sum_{i=1}^{d} \Big(2T^x_{F^{[3]}_{2,d}}(x, D_i x, D_i x) + T^x_{F^{[2]}_{2,d}}(a_i, D_i x) \Big) + T^x_{F^{[2]}_{2,d}}(x, \Delta x) \\
&+ T^x_{F^{[1]}_{2,d}}(a) + \sum_{i=1}^{d} \frac{1}{d} \Big(4T^x_{F^{[4]}_{2,d}}(x, D_i x, x, D_i x) + 4T^x_{F^{[3]}_{2,d}}(x, D_i x, D_i x) \\
&+ 8T^x_{F^{[4]}_{2,d}}(x, x, D_i x, D_i x) + 2T^x_{F^{[3]}_{2,d}}(x, D_i x, a_i) + 2T^x_{F^{[2]}_{2,d}}(x, D_i a_i) \\
&+ 2T^x_{F^{[3]}_{2,d}}(x, a_i, D_i x) + 2T^x_{F^{[3]}_{2,d}}(a_i, x, D_i x) + T^x_{F^{[2]}_{2,d}}(a_i, a_i) \Big) \\
&+ \frac{4}{d} T^x_{F^{[3]}_{2,d}}(x, x, \Delta x).
\end{aligned}$$

Deriving the above formula from our main theorem is quite straightforward; Section 8 contains an explicit proof for convenience of the reader.

In fact, the same can be done for any order k in a simple manner.

Corollary 3.7. *For any $d \in \mathbb{N}_{\geq 2}$, $k \in 2\mathbb{Z}_+$, and P acting in $L_2(\mathbb{T}^d_\theta)$ of the form (1.2) for positive invertible x, an expression for the k^{th} order local invariant $I_k(P)$ can be computed by the accompanying python program (cf. Appendix A). This expression consists of a finite amount of terms of the form*

$$c\pi^{\frac{d}{2}} T^x_{F^{[m]}_{k,d}}(D^{\alpha_1} b_1, \ldots, D^{\alpha_m} b_m),$$

where $m \in \mathbb{N}$, $c \in \mathbb{Q}$, $\alpha_j \in \mathbb{Z}^d_+$ and $b_j \in \{x, a_1, \ldots, a_d, a\}$. E.g., I_4 has 1046 terms and I_6 has 140845 terms in Einstein notation (i.e., not counting sums over indices $i_j = 1, \ldots, d$).

For specific P and k, the above expressions can yield remarkably elegant results. As an example we shall focus on $k = 2$ and the case $P = \lambda_l(x^{1/2})\Delta\lambda_l(x^{1/2})$, which corresponds to the Laplacian 'on functions' (see [7,13] for terminology) of the conformally deformed non-commutative 2-torus. In this case (and in fact in the analogous case for every $d \geq 2$) we obtain an expression for $I_2(P)$ that is arguably neater than the expressions one finds in the literature (cf. [7]).[2]

Theorem 3.8. *Let $d \geq 2$ and consider $P = \lambda_l(x^{\frac{1}{2}})\Delta\lambda_l(x^{\frac{1}{2}})$ acting in $L_2(\mathbb{T}^d_\theta)$ for a positive invertible $x \in C^\infty(\mathbb{T}^d_\theta)$. The second order local invariant of P is given by*

$$-\pi^{-\frac{d}{2}} I_2(P) = T^x_\Phi(\Delta x) + \sum_{i=1}^{d} T^x_\Psi(D_i x, D_i x),$$

where Φ and Ψ are expressed in terms of divided differences as

$$\Phi(\alpha_0, \alpha_1) = \frac{2(\alpha_0\alpha_1)^{\frac{1}{2}}}{d} \cdot \frac{\alpha_0 F^{[2]}_{2,d}(\alpha_0, \alpha_0, \alpha_1) - \alpha_1 F^{[2]}_{2,d}(\alpha_0, \alpha_1, \alpha_1)}{\alpha_1 - \alpha_0},$$

$$\Psi(\alpha_0, \alpha_1, \alpha_2) = -\frac{4}{d}\frac{(\alpha_0\alpha_2)^{\frac{1}{2}}}{\alpha_1^{2+\frac{d}{2}}} g^{[3]}\left(\frac{\alpha_0}{\alpha_1}, \frac{\alpha_0}{\alpha_1}, \frac{\alpha_2}{\alpha_1}, \frac{\alpha_2}{\alpha_1}\right), \quad g(\alpha) = F_{2,d}(\alpha) + F^{[1]}_{2,d}(1, \alpha),$$

for all $\alpha_0, \alpha_1, \alpha_2, \alpha > 0$.

Multiple operator integrals can also serve as a stepping stone towards the modular functional calculus ubiquitous in the literature since [4,7,8]. Indeed, from the above formula one can derive the most basic main results of [7,13] as a corollary, namely the functions $K_0(s)$ and $H_0(s,t)$ from [7]. This derivation is done in Section 9.

In fact, as our main result holds for arbitrary d and k, many more 'modular formulas' are now within easy reach. As a quick example, if $k = 2$ and $d \geq 3$ is arbitrary, then Theorem 9.4 (which can be derived from Theorem 3.8 or directly from our main theorem) shows how the function

$$K^d_0(s) = \frac{2}{d} \cdot \frac{-1 - e^{(1-\frac{d}{2})s} + \frac{e^{(1-d/2)s}-1}{1-d/2}\coth\left(\frac{s}{2}\right)}{s\sinh\left(\frac{s}{2}\right)}$$

replaces the function $K_0(s)$ of [7, eq. (2)] when passing to arbitrary dimension. Moreover, one immediately recovers the function $K_0(s)$ of [7] by taking $d \to 2$ in the above formula.

[2] Theorem 3.8 is just one of many possible applications of our main theorem. An unwieldy but explicit expression for I_2 of the full Laplacian of a conformally deformed noncommutative d-torus (either in terms of multiple operator integrals or in terms of modular functional calculus, see Section 9) follows straightforwardly from Corollary 3.6. A simplification of it in the spirit of Theorem 3.8 and/or a geometric interpretation of it would be an interesting follow-up research.

The recursive formula of Theorem 3.3 bears similarity to some of the formulas in [24–26]. Indeed, we show how to recover a key result from [24] from our main theorem in Theorem 10.3, thus finally bridging the gap between the commutative and non-commutative approaches.

4. Groundwork

Lemma 4.1. *The map* $\mathbf{T} : \mathcal{X}^{\times n} \to C^\infty(\mathbb{T}^d_\theta)$ *of Definition 3.1 is well defined.*

Proof. It suffices to show that the expression defining

$$\mathbf{T}_f^{x,n}(\mathbf{B}_1, \ldots, \mathbf{B}_{k-1}, \mathbf{B}_k\mathbf{D}_i\mathbf{D}_j, b_{k+1}, \ldots, b_n) \tag{4.1}$$

equals the expression defining

$$\mathbf{T}_f^{x,n}(\mathbf{B}_1, \ldots, \mathbf{B}_{k-1}, \mathbf{B}_k\mathbf{D}_j\mathbf{D}_i, b_{k+1}, \ldots, b_n). \tag{4.2}$$

By induction, one can show that (4.1) is equal to a long expression involving D_i and D_j occurring in the arguments after $\mathbf{B}_1, \ldots, \mathbf{B}_k$ in one of the following forms

$$\begin{aligned}
\ldots, D_i x, \ldots, D_j x, \ldots, \qquad & \ldots, D_j x, \ldots, D_i x, \ldots, \\
\ldots, D_i b_l, \ldots, D_j x, \ldots, \qquad & \ldots, D_j b_l, \ldots, D_i x, \ldots, \\
\ldots, D_i x, \ldots, D_j b_m, \ldots, \qquad & \ldots, D_j x, \ldots, D_i b_m, \ldots, \\
\ldots, D_i b_l, \ldots, D_j b_m, \ldots, \qquad & \ldots, D_j b_l, \ldots, D_i b_m, \ldots, \\
\ldots, D_i D_j x, \ldots, \qquad & \ldots, D_i D_j b_l, \ldots,
\end{aligned}$$

where the dots signify the list of other arguments $b_{k+1}, \ldots, b_n$, cut up at arbitrary places. One sees that the first 8 instances are in bijection with one another after swapping i and j. The last 2 instances are invariant under swapping i and j because $D_iD_j = D_jD_i$. Hence (4.1) is equal to (4.2). □

4.1. The results of our companion paper

In our companion paper [43] the existence of the asymptotic expansion was proven for the present general class of operators P (in fact, for an even more general assumption on the scalar symbol), and a formula was given for $I_k(P)$. However, this formula was not explicit.

As in [43], this formula is stated as a definition of $I_k(P)$ for all P of the form (1.2) with x self-adjoint and invertible. If P is in addition self-adjoint, this definition of $I_k(P)$ coincides with the definition in the introduction (see Theorem 4.7 below).

Definition 4.2. For $s \in \mathbb{R}^d$, we define

$$V(s) := \sum_{i=1}^{d} s_i A_i,$$
$$A_i := 2\lambda_l(x) D_i + \lambda_l(a_i), \quad 1 \le i \le d,$$

as linear operators $C^\infty(\mathbb{T}_\theta^d) \to L_2(\mathbb{T}_\theta^d)$ acting (densely) in $L_2(\mathbb{T}_\theta^d)$.

As x is positive and invertible, $x|s|^2 + z \in C^\infty(\mathbb{T}_\theta^d)$ is invertible in $L_\infty(\mathbb{T}_\theta^d)$ for every $z \in \mathbb{C}\backslash\mathbb{R}_-$. As $C^\infty(\mathbb{T}_\theta^d)$ is stable under holomorphic functional calculus, we have $(x|s|^2 + z)^{-1} \in C^\infty(\mathbb{T}_\theta^d)$.

Definition 4.3. Let $\mathscr{A} \subseteq \mathbb{N}$. For every $z \in \mathbb{C}\backslash\mathbb{R}_-$ and every $s \in \mathbb{R}^d$, set $f_0^{\mathscr{A}}(s,z) := 1$ and

$$f_m^{\mathscr{A}}(s,z) := W_j^{\mathscr{A}}(s)\Big(\frac{1}{x|s|^2 + z} f_{m-1}^{\mathscr{A}}(s,z)\Big), \quad m \ge 1,$$

where (cf. (3.5))

$$W_j^{\mathscr{A}}(s) := \begin{cases} V(s) & (j \in \mathscr{A}); \\ P & (j \notin \mathscr{A}). \end{cases} \tag{4.3}$$

Definition 4.4. For every $z \in \mathbb{C}\backslash\mathbb{R}_-$ every $s \in \mathbb{R}^d$ and every $k \in \mathbb{Z}_+$ we set

$$\mathrm{corr}_k(s,z) := (x|s|^2 + z)^{-1} \sum_{\frac{k}{2} \le m \le k} (-1)^m \sum_{\substack{\mathscr{A} \subseteq \{1,\cdots,m\} \\ |\mathscr{A}| = 2m-k}} f_m^{\mathscr{A}}(s,z).$$

Definition 4.5. For every $s \in \mathbb{R}^d$ and every $k \in \mathbb{Z}_+$ we set

$$\mathrm{Corr}_k(s) := \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{corr}_k(s, i\lambda) e^{i\lambda}\, d\lambda.$$

Here and throughout this paper, $\int_{-\infty}^{\infty} := \lim_{N\to\infty} \int_{-N}^{N}$. In the case above, the limit is with respect to the weak operator topology. The distinction between $\int_{-\infty}^{\infty}$ and the Lebesgue integral $\int_{\mathbb{R}}$ is only relevant in the case $k = 0$.

Definition 4.6. For every $k \in \mathbb{Z}_+$, we define

$$I_k(P) := \int_{\mathbb{R}^d} \mathrm{Corr}_k(s)\, ds,$$

as a weak integral in $L_\infty(\mathbb{T}_\theta^d)$.

Theorem 1.2 in [43] asserts the following.

Theorem 4.7. *If P is self-adjoint acting in $L_2(\mathbb{T}_\theta^d)$ of the form (1.2) for x positive and invertible, then (1.1) holds with $\{I_k(P)\}_{k\geq 0}$ as in Notation 4.6, and $I_k(P) \in C^\infty(\mathbb{T}_\theta^d)$ for all $k \geq 0$.*

In the next three sections we will rewrite the above definition into a computable formula for $I_k(P)$, and thus prove our main theorem.

5. Recursion at the level of symbols

Recall that $\mathcal{X} := \operatorname{span}\{b\mathbf{D}^\alpha \mid b \in C^\infty(\mathbb{T}_\theta^d), \alpha \in \mathbb{Z}_+^d\}$, a free $C^\infty(\mathbb{T}_\theta^d)$-module. Similarly, let $X := \{\lambda_l(b)D^\alpha : C^\infty(\mathbb{T}_\theta^d) \to C^\infty(\mathbb{T}_\theta^d) \mid b \in C^\infty(\mathbb{T}_\theta^d), \alpha \in \mathbb{Z}_+^d\}$ be the $C^\infty(\mathbb{T}_\theta^d)$-module generated by the operators $D^\alpha = D_1^{\alpha_1} \cdots D_d^{\alpha_d}$, $\alpha \in \mathbb{Z}_+^d$, seen here simply as linear functions from $C^\infty(\mathbb{T}_\theta^d)$ to $C^\infty(\mathbb{T}_\theta^d)$. We define a $C^\infty(\mathbb{T}_\theta^d)$-module homomorphism $\pi : \mathcal{X} \to X$ by linear extension of

$$\pi(b\mathbf{D}^\alpha) := \lambda_l(b)D^\alpha. \tag{5.1}$$

Fix a positive invertible $x \in C^\infty(\mathbb{T}_\theta^d)$. We define multilinear mappings $S_{s,z}^m : \mathcal{X}^{\times m} \to C^\infty(\mathbb{T}_\theta^d)$ for every $m \in \mathbb{N}$, $s \in \mathbb{R}^d \setminus \{0\}$ and $z \in \mathbb{C} \setminus \mathbb{R}_-$ by

$$\begin{aligned} &S_{s,z}^m(\mathbf{B}_1, \ldots, \mathbf{B}_m) := \\ &(-1)^m |s|^{2m} \frac{1}{x|s|^2 + z} \pi(\mathbf{B}_1)\Big(\frac{1}{x|s|^2 + z} \cdots \pi(\mathbf{B}_m)\Big(\frac{1}{x|s|^2 + z}\Big) \cdots\Big), \end{aligned} \tag{5.2}$$

for all $\mathbf{B}_1, \ldots, \mathbf{B}_m \in \mathcal{X}$. The above expression is well-defined because $(x|s|^2 + z)^{-1} \in C^\infty(\mathbb{T}_\theta^d)$ and elements of X preserve $C^\infty(\mathbb{T}_\theta^d)$. By defining $S_{s,z}^m$ as above, we neatly separate the recursive structure from the analysis in the proof of our main theorem. In the following subsection we show that $S_{s,z}^m$ satisfies the same recursive properties as $\mathbf{T}_f^{x,m}$ does by Definition 3.1 (i.e., (3.1) and (3.2)). Relating $S_{s,z}^n(b_1, \ldots, b_n)$ to $\mathbf{T}_f^{x,n}(b_1, \ldots, b_n)$ for $b_i \in C^\infty(\mathbb{T}_\theta^d)$ (i.e., relating the two base cases of the respective recursions) involves some heavy analysis, and is done in Section 6.

5.1. Recursive formula for $S_{s,z}$

The following two lemmas show how expressions of the form $S_{s,z}^m(\mathbf{B}_1, \ldots, \mathbf{B}_m)$ (where $\mathbf{B}_i \in \mathcal{X}$) can be rewritten in terms of expressions of the form $S_{s,z}^n(b_1, \ldots, b_n)$, where $b_i \in C^\infty(\mathbb{T}_\theta^d)$ and $n \geq m$.

Lemma 5.1. *Let $k, m \in \mathbb{N}$, $k < m$, $\mathbf{B}_1, \ldots, \mathbf{B}_k \in \mathcal{X}$, $b_{k+1}, \ldots, b_m \in C^\infty(\mathbb{T}_\theta^d) \subseteq \mathcal{X}$, and $i \in \{1, \ldots, d\}$. For all $s \in \mathbb{R}^d \setminus \{0\}$ and $z \in \mathbb{C} \setminus \mathbb{R}_-$ we have*

$$
\begin{aligned}
S^m_{s,z}(\mathbf{B}_1,\ldots,\mathbf{B}_{k-1},\mathbf{B}_k\mathbf{D}_i,b_{k+1},\ldots,b_m) &= S^{m+1}_{s,z}(\mathbf{B}_1,\ldots,\mathbf{B}_k,D_ix,b_{k+1},\ldots,b_m)\\
&\quad + S^m_{s,z}(\mathbf{B}_1,\ldots,\mathbf{B}_k,D_ib_{k+1},b_{k+2},\ldots,b_m)\\
&\quad + S^m_{s,z}(\mathbf{B}_1,\ldots,\mathbf{B}_k,b_{k+1}\mathbf{D}_i,b_{k+2},\ldots,b_m).
\end{aligned}
$$

Proof. We first note that from $D_i(u\cdot u^{-1})=0$ it follows that

$$
D_i(u^{-1}) = -u^{-1}\cdot D_iu\cdot u^{-1}.
$$

Thusly, we obtain

$$
D_i\Big(\frac{1}{x|s|^2+z}\Big) = -|s|^2\frac{1}{x|s|^2+z}(D_ix)\frac{1}{x|s|^2+z}.
$$

By the latter equality and the Leibniz rule we obtain, for any $k\in\mathbb{Z}$,

$$
\begin{aligned}
&\pi(\mathbf{D}_i)\Big(\frac{1}{x|s|^2+z}b_{k+1}\frac{1}{x|s|^2+z}\cdots b_m\frac{1}{x|s|^2+z}\Big)\\
&\quad = D_i\Big(\frac{1}{x|s|^2+z}b_{k+1}\frac{1}{x|s|^2+z}\cdots b_m\frac{1}{x|s|^2+z}\Big)\\
&\quad = -|s|^2\frac{1}{x|s|^2+z}D_ix\frac{1}{x|s|^2+z}b_{k+1}\frac{1}{x|s|^2+z}\cdots b_n\frac{1}{x|s|^2+z}\\
&\qquad + \frac{1}{x|s|^2+z}D_ib_{k+1}\frac{1}{x|s|^2+z}b_{k+2}\frac{1}{x|s|^2+z}\cdots b_n\frac{1}{x|s|^2+z}\\
&\qquad + \frac{1}{x|s|^2+z}b_{k+1}D_i\Big(\frac{1}{x|s|^2+z}b_{k+2}\frac{1}{x|s|^2+z}\cdots b_n\frac{1}{x|s|^2+z}\Big)\\
&\quad = -|s|^2\frac{1}{x|s|^2+z}D_ix\frac{1}{x|s|^2+z}b_{k+1}\frac{1}{x|s|^2+z}\cdots b_n\frac{1}{x|s|^2+z}\\
&\qquad + \frac{1}{x|s|^2+z}D_ib_{k+1}\frac{1}{x|s|^2+z}b_{k+2}\frac{1}{x|s|^2+z}\cdots b_n\frac{1}{x|s|^2+z}\\
&\qquad + \frac{1}{x|s|^2+z}\pi(b_{k+1}\mathbf{D}_i)\Big(\frac{1}{x|s|^2+z}b_{k+2}\frac{1}{x|s|^2+z}\cdots b_n\frac{1}{x|s|^2+z}\Big).
\end{aligned}
$$

After multiplying both sides by $(-1)^{m-k}|s|^{2(m-k)}$, the above equality becomes

$$
\begin{aligned}
\pi(\mathbf{D}_i)\Big(S^{m-k}_{s,z}(b_{k+1},\ldots,b_m)\Big) =& S^{m-k+1}_{s,z}(D_ix,b_{k+1},\ldots,b_m)\\
&+ S^{m-k}_{s,z}(D_ib_{k+1},b_{k+2},\ldots,b_m)\\
&+ S^{m-k}_{s,z}(b_{k+1}\mathbf{D}_i,b_{k+2},\ldots,b_m).
\end{aligned}
\tag{5.3}
$$

As

$$S^m_{s,z}(\mathbf{B}_1,\ldots,\mathbf{B}_k,\mathbf{B}_{k+1},\ldots,\mathbf{B}_m)$$
$$= (-1)^k|s|^{2k}\frac{1}{x|s|^2+z}\pi(\mathbf{B}_1)\Big(\cdots\frac{1}{x|s|^2+z}\pi(\mathbf{B}_k)\Big(S^{m-k}_{s,z}(\mathbf{B}_{k+1},\ldots,\mathbf{B}_m)\Big)\cdots\Big),$$

the lemma follows from (5.3). □

Lemma 5.2. *Let $m\in\mathbb{N}$, $\mathbf{B}_1,\ldots,\mathbf{B}_m\in\mathcal{X}$ and $i\in\{1,\ldots,d\}$. For all $s\in\mathbb{R}^d\setminus\{0\}$ and $z\in\mathbb{C}\setminus\mathbb{R}_-$ we have*

$$S^m_{s,z}(\mathbf{B}_1,\ldots,\mathbf{B}_{m-1},\mathbf{B}_m\mathbf{D}_i) := S^{m+1}_{s,z}(\mathbf{B}_1,\ldots,\mathbf{B}_m,D_ix).$$

Proof. This is an easier version of the proof of Lemma 5.1. □

6. Analytical results on multiple operator integrals

The purpose of this section is to prove the following theorem.

Theorem 6.1. *Let $x\in C^\infty(\mathbb{T}^d_\theta)$ be positive and invertible. For every $n\in\mathbb{N}$, $b_1,\ldots,b_n\in C^\infty(\mathbb{T}^d_\theta)$, and every $k\in 2\mathbb{Z}_+$ such that $2n-k\geq 0$, we have*

$$\frac{1}{2\pi}\int_{\mathbb{R}^d}\Big(\int_{-\infty}^{\infty}|s|^{-k}S^n_{s,i\lambda}(b_1,\ldots,b_n)e^{i\lambda}d\lambda\Big)ds = (-1)^{\frac{k}{2}}\pi^{\frac{d}{2}}\cdot T^x_{F^{[n]}_{k,d}}(b_1,\ldots,b_n),$$

where $F_{k,d}$ is any $\frac{k}{2}^{th}$ primitive of $\alpha\mapsto\alpha^{-\frac{d}{2}}$.

For any open interval $I\subseteq\mathbb{R}$ and any $n\in\mathbb{N}$ we will use the space

$$\dot{W}^{n,2}(I) := \{f\in\mathcal{S}'(I):\ f^{(n)}\in L_2(I)\}$$

(where $\mathcal{S}'(I)$ denotes the tempered distributions on I) with associated seminorm

$$\|f\|_{\dot{W}^{n,2}(I)} := \|f^{(n)}\|_{L_2(I)}.$$

By slight abuse of notation, we denote by $(\dot{W}^{n,2}\cap\dot{W}^{n+1,2})(I)$ the space of equivalence classes of functions in $\dot{W}^{n,2}(I)\cap\dot{W}^{n+1,2}(I)$ modulo polynomials of degree at most $n-1$. We omit the notation for 'the equivalence class of'. We equip $(\dot{W}^{n,2}\cap\dot{W}^{n+1,2})(I)$ with the norm

$$\|f\|_{(\dot{W}^{n,2}\cap\dot{W}^{n+1,2})(I)} := \|f^{(n)}\|_{L_2(I)} + \|f^{(n+1)}\|_{L_2(I)}.$$

This space $(\dot{W}^{n,2}\cap\dot{W}^{n+1,2})(I)$ is a Banach space, as can be shown by standard techniques. Note also that any $f\in\dot{W}^{n,2}(I)$ is a continuous function, because $f^{(n)}$ is locally integrable. Hence, any representative of a class in $(\dot{W}^{n,2}\cap\dot{W}^{n+1,2})(I)$ is a continuous function.

Lemma 6.2. *Let $x \in L_\infty(\mathbb{T}^d_\theta)$ be self-adjoint and let I be an open interval containing* $\mathrm{spec}(x)$. *Let f be a Schwartz function on $\mathbb{R}$. For all $b_1, \ldots, b_n \in L_\infty(\mathbb{T}^d_\theta)$ we have*

$$\|T^x_{f^{[n]}}(b_1, \cdots, b_n)\|_\infty \leq c_{n,x,I}\|f\|_{(\dot{W}^{n,2}\cap\dot{W}^{n+1,2})(I)}\prod_{l=1}^n \|b_l\|_\infty.$$

Proof. Let $J = [\inf \mathrm{spec}(x), \sup \mathrm{spec}(x)] \subseteq I$. Let ϕ be a smooth function supported in I such that ϕ equals 1 on J. We have

$$f^{[n]}(\alpha_0, \cdots, \alpha_n) = \int\limits_{S^n} f^{(n)}\Big(\sum_{j=0}^n \lambda_j\alpha_j\Big)d\lambda,$$

where the integration is taken with respect to the standard measure on the simplex $S^n = \{\lambda \in \mathbb{R}^{n+1}_{\geq 0} : \sum_{j=0}^n \lambda_j = 1\}$. If $\alpha_0, \cdots, \alpha_n \in \mathrm{spec}(x)$, then $\sum_{j=0}^n \lambda_j\alpha_j \in J$. Therefore, denoting the Fourier transform of the Schwartz function $f^{(n)}\phi$ by $\widehat{(f^{(n)}\phi)}$, we have

$$\begin{aligned} f^{[n]}(\alpha_0, \cdots, \alpha_n) &= \int\limits_{S^n} (f^{(n)}\phi)\Big(\sum_{j=0}^n \lambda_j\alpha_j\Big)d\lambda \\ &= \frac{1}{\sqrt{2\pi}}\int\limits_{S^n}\int\limits_{\mathbb{R}} \widehat{(f^{(n)}\phi)}(t)e^{it\lambda_0\alpha_0}\cdots e^{it\lambda_n\alpha_n}dt\,d\lambda, \end{aligned}$$

whenever $\alpha_0, \cdots, \alpha_n \in \mathrm{spec}(x)$. Thus,

$$\|T^x_{f^{[n]}}(b_1, \cdots, b_n)\|_\infty \leq \frac{1}{\sqrt{2\pi}n!}\|\widehat{(f^{(n)}\phi)}\|_{L_1(\mathbb{R})}\prod_{l=1}^n \|b_l\|_\infty.$$

Note that

$$\|\widehat{(f^{(n)}\phi)}\|_{L_1(\mathbb{R})} \leq \sqrt{2}\big(\|f^{(n)}\phi\|_{L_2(I)} + \|(f^{(n)}\phi)'\|_{L_2(I)}\big).$$

By the Leibniz rule, we deduce

$$\|\widehat{(f^{(n)}\phi)}\|_{L_1(\mathbb{R})} \leq \|f^{(n)}\|_{L_2(I)}(\|\phi\|_\infty + \|\phi'\|_\infty) + \|f^{(n+1)}\|_{L_2(I)}\|\phi\|_\infty.$$

Since ϕ depends only on x and I, the assertion follows. □

6.1. Integration over the symbol of a multiple operator integral

In this subsection we prove the following general result. We let $(\sigma_t f)(\alpha) := f(\alpha/t)$ denote the dilation operator.

Theorem 6.3. *Let $x \in \mathcal{B}(\mathcal{H})$ be positive and invertible. Let f be a Schwartz function on $\mathbb{R}$. Let $k \in 2\mathbb{Z}_+$ and $n \in \mathbb{N}$ be such that $2n \geq k$. For all $b_1, \ldots, b_n \in \mathcal{B}(\mathcal{H})$ we have*

$$\int_{\mathbb{R}^d} |s|^{-k} T^x_{(\sigma_{|s|^{-2}} f)^{[n]}}(b_1, \ldots, b_n)\, ds = \int_{\mathbb{R}^d} f^{(\frac{k}{2})}(|s|^2) ds \cdot T^x_{F^{[n]}_{k,d}}(b_1, \ldots, b_n),$$

where the left-hand side is a Bochner integral taking values in $\mathcal{B}(\mathcal{H})$, and $F_{k,d}$ is any $\frac{k}{2}^{th}$ primitive of $\alpha \mapsto \alpha^{-\frac{d}{2}}$ on $(0, \infty)$ (cf. Remark 3.4).

Lemma 6.4. *Let $k \in 2\mathbb{Z}_+$. Let f be a Schwartz function on $\mathbb{R}$ and let ϕ be a Schwartz function on $\mathbb{R}^d$ that equals 1 on a neighbourhood of 0. There exists a $\frac{k}{2}^{th}$ order primitive $F_{k,d}$ of $\alpha \mapsto \alpha^{-\frac{d}{2}}$ such that, for all $\alpha > 0$,*

$$\int_{\mathbb{R}^d} |s|^{-k} \Big(f(\alpha|s|^2) - \sum_{j=0}^{\frac{k}{2}-1} \frac{f^{(j)}(0)}{j!} (\alpha|s|^2)^j \cdot \phi(s) \Big) ds = \int_{\mathbb{R}^d} f^{(\frac{k}{2})}(|s|^2) ds \cdot F_{k,d}(\alpha).$$

Proof. The left-hand side integral converges because, as $s \to 0$, the expression between brackets is $\mathcal{O}(|s|^k)$. Similarly this integral converges after differentiating the integrand with respect to α. Denoting the left-hand side by $G(\alpha)$, we have

$$G^{(\frac{k}{2})}(\alpha) = \int_{\mathbb{R}^d} f^{(\frac{k}{2})}(\alpha|s|^2) ds = \alpha^{-\frac{d}{2}} \int_{\mathbb{R}^d} f^{(\frac{k}{2})}(|s|^2) ds.$$

Integrating $\frac{k}{2}$ times, we complete the proof. □

We have the following simple but powerful proposition.

Proposition 6.5. *Let $n \in \mathbb{N}$ and let $x \in \mathcal{B}(\mathcal{H})$ be self-adjoint. Let I be an open interval containing the spectrum of x. Let $s \mapsto h_s$ ($s \in \mathbb{R}^d$) be a Bochner integrable mapping taking values in $(\dot{W}^{n,2} \cap \dot{W}^{n+1,2})(I)$. Denote its Bochner integral by*

$$h = \int_{\mathbb{R}^d} h_s\, ds.$$

Then $h \in (\dot{W}^{n,2} \cap \dot{W}^{n+1,2})(I)$ and

$$\int_{\mathbb{R}^d} T^x_{h_s^{[n]}}(b_1, \ldots, b_n)\, ds = T^x_{h^{[n]}}(b_1, \ldots, b_n),$$

where the left-hand side is a Bochner integral with values in $\mathcal{B}(\mathcal{H})$.

Proof. By Lemma 6.2, the map

$$T : (\dot{W}^{n,2} \cap \dot{W}^{n+1,2})(I) \to \mathcal{B}(\mathcal{H}), \qquad f \mapsto T^x_{f^{[n]}}(b_1, \dots, b_n)$$

is a continuous linear map between Banach spaces. Hence $s \mapsto T(h_s)$ is Bochner integrable over $\mathbb{R}^d$ and $\int_{\mathbb{R}^d} T(h_s)ds = T(\int_{\mathbb{R}^d} h_s ds) = T(h)$. □

The function playing the role of h_s in the above proposition will be $h_s = |s|^{-k}(\sigma_{|s|^{-2}}f)|_I$, where $(\sigma_t f)(\alpha) := f(\alpha/t)$ denotes the dilation operator.

Lemma 6.6. *Let f be a Schwartz function on $\mathbb{R}$. Let I be a bounded open interval separated from 0. If $n \in \mathbb{N}$ and $k \in \mathbb{Z}_+$ satisfy $2n \geq k$, then the mapping*

$$s \mapsto |s|^{-k}(\sigma_{|s|^{-2}}f)|_I, \quad 0 \neq s \in \mathbb{R}^d.$$

is Bochner integrable to $(\dot{W}^{n,2} \cap \dot{W}^{n+1,2})(I)$.

Proof. It is immediate that

$$(|s|^{-k}\sigma_{|s|^{-2}}f)^{(n)} = |s|^{2n-k}\sigma_{|s|^{-2}}f^{(n)},$$
$$(|s|^{-k}\sigma_{|s|^{-2}}f)^{(n+1)} = |s|^{2n+2-k}\sigma_{|s|^{-2}}f^{(n+1)}.$$

These functions of s are continuous from $\mathbb{R}^d\setminus\{0\}$ to $L_2(\mathbb{R})$. Hence, the mapping $s \mapsto |s|^{-k}\sigma_{|s|^{-2}}f$ is continuous from $\mathbb{R}^d\setminus\{0\}$ to $(\dot{W}^{n,2} \cap \dot{W}^{n+1,2})(\mathbb{R})$. Hence, the mapping $s \mapsto |s|^{-k}(\sigma_{|s|^{-2}}f)|_I$ is continuous from $\mathbb{R}^d\setminus\{0\}$ to $(\dot{W}^{n,2} \cap \dot{W}^{n+1,2})(I)$, and therefore Bochner measurable.

Regarding absolute integrability, we have

$$\|(|s|^{-k}\sigma_{|s|^{-2}}f)^{(n)}\|_{L_2(I)} = |s|^{2n-k-1}\|f^{(n)}\|_{L_2(|s|^2 I)}\,,$$
$$\|(|s|^{-k}\sigma_{|s|^{-2}}f)^{(n+1)}\|_{L_2(I)} = |s|^{2n-k+1}\|f^{(n+1)}\|_{L_2(|s|^2 I)}\,.$$

Thus,

$$\||s|^{-k}\sigma_{|s|^{-2}}f\|_{(\dot{W}^{n,2}\cap\dot{W}^{n+1,2})(I)} \leq (|s|^{2n-k-1} + |s|^{2n-k+1})\|f\|_{(\dot{W}^{n,2}\cap\dot{W}^{n+1,2})(|s|^2 I)}\,.$$

As I is bounded away from 0, and f is Schwartz, the latter expression decays rapidly as $|s| \to \infty$. Moreover, as $2n - k \geq 0$, the factor $(|s|^{2n-k-1} + |s|^{2n-k+1})$ is of order $\mathcal{O}(|s|^{-1})$ as $|s| \to 0$. As I is bounded, and $f^{(n)}, f^{(n+1)}$ are continuous at 0, the factor $\|f\|_{(\dot{W}^{n,2}\cap\dot{W}^{n+1,2})(|s|^2 I)}$ is of order $\mathcal{O}(|s|)$ as $|s| \to 0$. Hence, the mapping $s \to |s|^{-k}(\sigma_{|s|^{-2}}f)|_I$ is absolutely integrable with respect to $(\dot{W}^{n,2} \cap \dot{W}^{n+1,2})(I)$ and the assertion follows. □

The following lemma gives a simplified expression for $h = \int_{\mathbb{R}^d} h_s\, ds$.

Lemma 6.7. *Let f be a Schwartz function on $\mathbb{R}$. Let $n \in \mathbb{N}$ and $k \in 2\mathbb{Z}_+$ such that $2n \geq k$. Let $I \subseteq (0, \infty)$ be a bounded open interval separated from 0. There exists a $\frac{k}{2}^{th}$ order primitive $F_{k,d}$ of $\alpha \mapsto \alpha^{-\frac{d}{2}}$ such that*

$$\int_{\mathbb{R}^d} |s|^{-k}(\sigma_{|s|^{-2}} f)|_I \, ds = \int_{\mathbb{R}^d} f^{(\frac{k}{2})}(|s|^2) ds \cdot F_{k,d}|_I \,,$$

where the left-hand side is a Bochner integral with values in $(\dot{W}^{n,2} \cap \dot{W}^{n+1,2})(I)$, and the right-hand side is interpreted as an element of $(\dot{W}^{n,2} \cap \dot{W}^{n+1,2})(I)$ as well.

Proof. Note that elements of $(\dot{W}^{n,2} \cap \dot{W}^{n+1,2})(I)$ are not exactly functions, but functions modulo polynomials of degree $< n$. For every $s \in \mathbb{R}^d \setminus \{0\}$, a particular representative of $|s|^{-k}(\sigma_{|s|^{-2}} f)|_I \in (\dot{W}^{n,2} \cap \dot{W}^{n+1,2})(I)$ is given by the function

$$\tilde{h}_s : I \to \mathbb{R}, \quad \tilde{h}_s(\alpha) := |s|^{-k} \Big(f(\alpha |s|^2) - \sum_{j=0}^{\frac{k}{2}-1} \frac{f^{(j)}(0)}{j!} (\alpha |s|^2)^j \cdot \phi(s) \Big).$$

Here, ϕ is a Schwartz function on $\mathbb{R}^d$ that equals 1 on a neighbourhood of 0. For a given $\alpha \in I$, we have

$$\big|\tilde{h}_s(\alpha)\big| = |s|^{-k} \cdot \mathcal{O}((|s|^2)^{\frac{k}{2}}) = \mathcal{O}(|s|^0).$$

Consequently, $s \mapsto \tilde{h}_s(\alpha)$ is integrable for every $\alpha \in I$, and the same holds for $s \mapsto \tilde{h}_s^{(j)}(\alpha)$, $j \leq n$. Recall that $s \mapsto |s|^{-k}(\sigma_{|s|^{-2}} f)|_I$ is Bochner integrable by Lemma 6.6. By using the definition of $(\dot{W}^{n,2} \cap \dot{W}^{n+1,2})(I)$, and subsequently using dominated convergence on $\alpha \mapsto \int \tilde{h}_s^{(j)}(\alpha) ds$, we obtain for almost every $\alpha \in I$,

$$\Big(\int_{\mathbb{R}^d} |s|^{-k}(\sigma_{|s|^{-2}} f)|_I \, ds \Big)^{(n)}(\alpha) = \int_{\mathbb{R}^d} \tilde{h}_s^{(n)}(\alpha) \, ds = \frac{d^n}{d\alpha^n} \Big(\int_{\mathbb{R}^d} \tilde{h}_s(\alpha) \, ds \Big).$$

Therefore, $\alpha \mapsto \int \tilde{h}_s(\alpha) ds$ is a representative of $\int |s|^{-k}(\sigma_{|s|^{-2}} f)|_I ds$. By Lemma 6.4 we have

$$\int_{\mathbb{R}^d} \tilde{h}_s(\alpha) \, ds = \int_{\mathbb{R}^d} f^{(\frac{k}{2})}(|s|^2) ds \cdot F_{k,d}(\alpha) \qquad (\alpha \in I),$$

and so the proof is complete. □

Proof of Theorem 6.3. Let $I = (\frac{1}{2} \inf \operatorname{spec}(x), 2 \sup \operatorname{spec}(x))$ and $h_s = |s|^{-k}(\sigma_{|s|^{-2}} f)|_I$, $s \in \mathbb{R}^d$. By Lemma 6.6, the conditions in Proposition 6.5 are met for the mapping $s \mapsto h_s$. Using Proposition 6.5 (and the fact that $g \mapsto T^x_{g^{[n]}}$ factors through $g \mapsto g|_I$) we have

$$\int_{\mathbb{R}^d} |s|^{-k} T^x_{(\sigma_{|s|^{-2}} f)^{[n]}}(b_1,\dots,b_n)\,ds = \int_{\mathbb{R}^d} T^x_{h_s^{[n]}}(b_1,\dots,b_n)\,ds$$
$$= T^x_{h^{[n]}}(b_1,\dots,b_n),$$

where

$$h = \int_{\mathbb{R}^d} h_s\,ds = \int_{\mathbb{R}^d} |s|^{-k}(\sigma_{|s|^{-2}} f)|_I\,ds.$$

By Lemma 6.7, we have

$$h = \int_{\mathbb{R}^d} f^{(\frac{k}{2})}(|s|^2)ds \cdot F_{k,d}|_I,$$

completing the proof. □

6.2. Integral formula relating the base cases of recursion

We can now prove the main theorem of Section 6.

Proof of Theorem 6.1. By definition of $S^n_{s,z}$ (equation (5.2)) we have, for $s \neq 0$,

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} |s|^{-k} S^n_{s,i\lambda}(b_1,\dots,b_n)e^{i\lambda}\,d\lambda$$
$$= (-1)^n|s|^{2n-k} \cdot \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{1}{x|s|^2+i\lambda} b_1 \frac{1}{x|s|^2+i\lambda} \cdots b_n \frac{1}{x|s|^2+i\lambda} e^{i\lambda}\,d\lambda.$$

Next,

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{1}{x|s|^2+i\lambda} b_1 \frac{1}{x|s|^2+i\lambda} \cdots b_n \frac{1}{x|s|^2+i\lambda} e^{i\lambda}d\lambda = T^x_{\Psi_s}(b_1,\dots,b_n),$$

where

$$\Psi_s(\alpha_0,\dots,\alpha_n) := \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{1}{\alpha_0|s|^2+i\lambda}\frac{1}{\alpha_1|s|^2+i\lambda} \cdots \frac{1}{\alpha_n|s|^2+i\lambda} e^{i\lambda}d\lambda,$$

for all $\alpha_0,\dots,\alpha_n > 0$. Let f be any Schwartz function that on $(0,\infty) \subseteq \mathbb{R}$ is defined by

$$f(\alpha) := \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{1}{\alpha+i\lambda} e^{i\lambda}d\lambda = e^{-\alpha}, \quad \alpha > 0.$$

Using the dilation $(\sigma_{|s|^{-2}}f)(\alpha) = f(|s|^2\alpha)$ and computing the divided differences of $\alpha \mapsto \frac{1}{\alpha|s|^2+i\lambda}$, we obtain

$$\Psi_s|_{(0,\infty)^{n+1}} = (-1)^n|s|^{-2n}(\sigma_{|s|^{-2}}f)^{[n]}|_{(0,\infty)^{n+1}}.$$

Therefore,

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} |s|^{-k}S^n_{s,i\lambda}(b_1,\dots,b_n)e^{i\lambda}d\lambda = |s|^{-k}T^x_{(\sigma_{|s|^{-2}}f)^{[n]}}(b_1,\dots,b_n). \tag{6.1}$$

By Theorem 6.3, and the fact that

$$\int_{\mathbb{R}^d} f^{(\frac{k}{2})}(|s|^2)ds = (-1)^{\frac{k}{2}}\int_{\mathbb{R}^d} e^{-|s|^2}\,ds = (-1)^{\frac{k}{2}}\pi^{\frac{d}{2}},$$

the assertion follows. □

7. Proof of the main theorem

We can summarise the previous section in the following way.

Corollary 7.1. *Let $x \in C^\infty(\mathbb{T}^d_\theta)$ be positive and invertible. For all $m \in \mathbb{N}$, $\mathbf{B}_1,\dots,\mathbf{B}_m \in \mathcal{X}$ and $k \in 2\mathbb{Z}_+$ such that $2m \geq k$, we have*

$$\frac{1}{2\pi}\int_{\mathbb{R}^d}\Big(\int_{-\infty}^{\infty} |s|^{-k}S^m_{s,i\lambda}(\mathbf{B}_1,\dots,\mathbf{B}_m)e^{i\lambda}d\lambda\Big)ds = (-1)^{\frac{k}{2}}\pi^{\frac{d}{2}}\cdot \mathbf{T}^{x,m}_{F_{k,d}}(\mathbf{B}_1,\dots,\mathbf{B}_m),$$

where $F_{k,d}$ is any $\frac{k}{2}^{th}$ primitive of $\alpha \mapsto \alpha^{-\frac{d}{2}}$.

Proof. This follows from the matching recursive properties of $\mathbf{T}^{x,m}_f$ (Definition 3.1) and $S^m_{s,z}$ (Lemmas 5.1 and 5.2) and the base case, Theorem 6.1. □

The above corollary is the final ingredient needed for the proof of our main theorem.

Proof of Theorem 3.3. By the definition of $I_k(P)$ as given in Section 4.1 we have

$$\begin{aligned} I_k(P) =& \frac{1}{2\pi}\int_{\mathbb{R}^d}\Big(\int_{-\infty}^{\infty}\sum_{\frac{k}{2}\leq m\leq k}(-1)^m\sum_{\substack{\mathscr{A}\subseteq\{1,\dots,m\}\\ |\mathscr{A}|=2m-k}}\frac{1}{x|s|^2+z} \\ &\cdot W^{\mathscr{A}}_1(s)\Big(\frac{1}{x|s|^2+z}\cdots W^{\mathscr{A}}_m(s)\Big(\frac{1}{x|s|^2+z}\Big)\cdots\Big)e^{i\lambda}\,d\lambda\Big)ds. \end{aligned}$$

Using the definition of $S^m_{s,z}$ (see (5.2)), and introducing elements $\mathbf{W}^{\mathscr{A}}_j(s) \in \mathcal{X}$ for which $\pi(\mathbf{W}^{\mathscr{A}}_j(s)) = W^{\mathscr{A}}_j(s)$, we rewrite the latter expression as

$$I_k(P) = \frac{1}{2\pi}\int_{\mathbb{R}^d}\Big(\int_{-\infty}^{\infty}\sum_{\frac{k}{2}\le m\le k}\sum_{\substack{\mathscr{A}\subseteq\{1,\dots,m\}\\ |\mathscr{A}|=2m-k}}\frac{1}{|s|^{2m}}S^m_{s,i\lambda}(\mathbf{W}^{\mathscr{A}}_1(s),\dots,\mathbf{W}^{\mathscr{A}}_m(s))e^{i\lambda}\,d\lambda\Big)ds.$$

By expressing $\mathbf{W}^{\mathscr{A}}_j(s)$ in terms of $\mathbf{W}^{\mathscr{A},\iota}_j$ of (3.5) (see also (4.3)) we obtain

$$S^m_{s,z}(\mathbf{W}^{\mathscr{A}}_1(s),\dots,\mathbf{W}^{\mathscr{A}}_m(s)) = \sum_{\iota:\mathscr{A}\to\{1,\dots,d\}}\Big(\prod_{j\in\mathscr{A}}s_{\iota(j)}\Big)S^m_{s,z}(\mathbf{W}^{\mathscr{A},\iota}_1,\dots,\mathbf{W}^{\mathscr{A},\iota}_m).$$

Thus,

$$\begin{aligned}I_k(P) =&\frac{1}{2\pi}\sum_{\frac{k}{2}\le m\le k}\sum_{\substack{\mathscr{A}\subseteq\{1,\dots,m\}\\ |\mathscr{A}|=2m-k}}\sum_{\iota:\mathscr{A}\to\{1,\dots,d\}}\\ &\qquad\int_{\mathbb{R}^d}\Big(\frac{\prod_{j\in\mathscr{A}}s_{\iota(j)}}{|s|^{2m}}\int_{-\infty}^{\infty}S^m_{s,i\lambda}(\mathbf{W}^{\mathscr{A},\iota}_1,\dots,\mathbf{W}^{\mathscr{A},\iota}_m)e^{i\lambda}\,d\lambda\Big)ds.\end{aligned}$$

Since the mapping

$$s\mapsto\int_{-\infty}^{\infty}S^m_{s,i\lambda}(\mathbf{W}^{\mathscr{A},\iota}_1,\dots,\mathbf{W}^{\mathscr{A},\iota}_m)e^{i\lambda}d\lambda,\quad s\in\mathbb{R}^d,$$

is a function of $|s|$, we can apply the general formula

$$\begin{aligned}\int_{\mathbb{R}^d}\frac{s^n}{|s|^{|n|_1}}g(|s|)ds &= \frac{1}{\mathrm{Vol}(\mathbb{S}^{d-1})}\int_{\mathbb{S}^{d-1}}u^n du\cdot\int_{\mathbb{R}^d}g(|s|)ds \\ &\equiv c_d^{(\iota)}\int_{\mathbb{R}^d}g(|s|)ds,\end{aligned}\tag{7.1}$$

for $n\in\mathbb{Z}^d_+$ satisfying $n_j = |\iota^{-1}(\{j\})|$, and find that

$$\begin{aligned}I_k(P) = &\sum_{\frac{k}{2}\le m\le k}\sum_{\substack{\mathscr{A}\subseteq\{1,\dots,m\}\\ |\mathscr{A}|=2m-k}}\sum_{\iota:\mathscr{A}\to\{1,\dots,d\}}c_d^{(\iota)}\frac{1}{2\pi}\\ &\cdot\int_{\mathbb{R}^d}\Big(\int_{-\infty}^{\infty}|s|^{-k}S^m_{s,i\lambda}(\mathbf{W}^{\mathscr{A},\iota}_1,\dots,\mathbf{W}^{\mathscr{A},\iota}_m)e^{i\lambda}\,d\lambda\Big)ds.\end{aligned}$$

By applying Corollary 7.1, we obtain our main theorem. □

8. The case $k = 2$: 'scalar curvature'

Although the formula in Corollary 3.6 can be obtained directly from the computer (as done in Appendix A) we will first give an explicit proof by hand, demonstrating the simplicity of the algorithm. We fix $d \in \mathbb{N}_{\geq 2}$ and $F_{2,d}$ as in Remark 3.4

Lemma 8.1. *For any P of the form (1.2) with positive invertible x, (3.7) gives*

$$-\pi^{-\frac{d}{2}} I_2(P) = \mathbf{T}^{x,1}_{F_{2,d}}(\mathbf{P}) + \frac{1}{d}\sum_{i=1}^{d} \mathbf{T}^{x,2}_{F_{2,d}}(\mathbf{A}_i, \mathbf{A}_i). \tag{8.1}$$

Proof. Our main theorem (Theorem 3.3) in the case $k = 2$ becomes

$$I_2(P) = -\sum_{1\leq m\leq 2} \sum_{\substack{\mathscr{A}\subseteq\{1,\dots,m\}\\ |\mathscr{A}|=2m-2}} \sum_{\iota:\mathscr{A}\to\{1,\dots,d\}} c_d^{(\iota)} \pi^{\frac{d}{2}} \mathbf{T}^{x,m}_{F_{2,d}}(\mathbf{W}_1^{\mathscr{A},\iota}, \dots, \mathbf{W}_m^{\mathscr{A},\iota}). \tag{8.2}$$

If $m = 1$ then $|\mathscr{A}| = 2m - 2$ implies $\mathscr{A} = \emptyset$; we then denote the unique function $\iota : \mathscr{A} \to \{1,\dots,d\}$ by $\iota = \emptyset$. If $m = 2$ then $|\mathscr{A}| = 2m - 2$ implies $\mathscr{A} = \{1, 2\}$; we then identify $\iota : \{1, 2\} \to \{1,\dots,d\}$ with $(i, j) = (\iota(1), \iota(2))$ for $i, j \in \{1,\dots,d\}$. We obtain

$$\begin{aligned} I_2(P) &= -c_d^{(\emptyset)} \pi^{\frac{d}{2}} \mathbf{T}^{x,1}_{F_{2,d}}(\mathbf{W}_1^{\emptyset,\emptyset}) - \sum_{i,j=1}^{d} c_d^{(i,j)} \pi^{\frac{d}{2}} \mathbf{T}^{x,2}_{F_{2,d}}(\mathbf{W}_1^{\mathscr{A},(i,j)}, \mathbf{W}_2^{\mathscr{A},(i,j)}) \\ &= -c_d^{(\emptyset)} \pi^{\frac{d}{2}} \mathbf{T}^{x,1}_{F_{2,d}}(\mathbf{P}) - \sum_{i,j=1}^{d} c_d^{(i,j)} \pi^{\frac{d}{2}} \mathbf{T}^{x,2}_{F_{2,d}}(\mathbf{A}_i, \mathbf{A}_j). \end{aligned}$$

Remark 3.5 gives $c_d^{(\emptyset)} = \frac{(d-2)!!}{(0+d-2)!!} = 1$ and $c_d^{(i,j)} = \delta_{i,j} \frac{(d-2)!!}{(2+d-2)!!} = \delta_{i,j} \frac{1}{d}$. We therefore obtain (8.1). □

Proof of Corollary 3.6. We work out the first term on the right hand side of (8.1) by using (3.6) and Definition 3.1. In a similar way to Example 3.2 we obtain

$$\begin{aligned} \mathbf{T}^{x,1}_{F_{2,d}}(\mathbf{P}) =& \mathbf{T}^{x,1}_{F_{2,d}}(x\sum_{i=1}^{d} \mathbf{D}_i^2 + \sum_{i=1}^{d} a_i \mathbf{D}_i + a) \\ =& \sum_{i=1}^{d} \Big(\mathbf{T}^{x,2}_{F_{2,d}}(x\mathbf{D}_i, D_i x) + \mathbf{T}^{x,2}_{F_{2,d}}(a_i, D_i x)\Big) + \mathbf{T}^{x,1}_{F_{2,d}}(a) \\ =& \sum_{i=1}^{d} \Big(\mathbf{T}^{x,3}_{F_{2,d}}(x, D_i x, D_i x) + \mathbf{T}^{x,2}_{F_{2,d}}(x, D_i D_i x) + \mathbf{T}^{x,2}_{F_{2,d}}(x, (D_i x)\mathbf{D}_i) \\ &+ T^{x}_{F^{[2]}_{2,d}}(a_i, D_i x)\Big) + T^{x}_{F^{[1]}_{2,d}}(a) \end{aligned}$$

$$= \sum_{i=1}^{d} \Big(2T^x_{F^{[3]}_{2,d}}(x, D_i x, D_i x) + T^x_{F^{[2]}_{2,d}}(a_i, D_i x) \Big) + T^x_{F^{[2]}_{2,d}}(x, \Delta x) + T^x_{F^{[1]}_{2,d}}(a).$$

Once you get the hang of it, working out the second term is child's play. For all $i \in \{1, \ldots, d\}$ we obtain

$$\begin{aligned}
&\mathbf{T}^{x,2}_{F_{2,d}}(\mathbf{A}_i, \mathbf{A}_i) \\
&= \mathbf{T}^{x,2}_{F_{2,d}}(2x\mathbf{D}_i + a_i, 2x\mathbf{D}_i + a_i) \\
&= 4\mathbf{T}^{x,3}_{F_{2,d}}(x\mathbf{D}_i, x, D_i x) + 2\mathbf{T}^{x,2}_{F_{2,d}}(x\mathbf{D}_i, a_i) \\
&\quad + 2T^x_{F^{[3]}_{2,d}}(a_i, x, D_i x) + T^x_{F^{[2]}_{2,d}}(a_i, a_i) \\
&= 4\Big(\mathbf{T}^{x,4}_{F_{2,d}}(x, D_i x, x, D_i x) + \mathbf{T}^{x,3}_{F_{2,d}}(x, D_i x, D_i x) + \mathbf{T}^{x,4}_{F_{2,d}}(x, x, D_i x, D_i x) \\
&\quad + \mathbf{T}^{x,3}_{F_{2,d}}(x, x, D_i D_i x) + \mathbf{T}^{x,4}_{F_{2,d}}(x, x, D_i x, D_i x) \Big) + 2\Big(\mathbf{T}^{x,3}_{F_{2,d}}(x, D_i x, a_i) \\
&\quad + \mathbf{T}^{x,2}_{F_{2,d}}(x, D_i a_i) + \mathbf{T}^{x,3}_{F_{2,d}}(x, a_i, D_i x) \Big) + 2T^x_{F^{[3]}_{2,d}}(a_i, x, D_i x) + T^x_{F^{[2]}_{2,d}}(a_i, a_i) \\
&= 4T^x_{F^{[4]}_{2,d}}(x, D_i x, x, D_i x) + 4T^x_{F^{[3]}_{2,d}}(x, D_i x, D_i x) + 8T^x_{F^{[4]}_{2,d}}(x, x, D_i x, D_i x) \\
&\quad + 4T^x_{F^{[3]}_{2,d}}(x, x, D_i^2 x) + 2T^x_{F^{[3]}_{2,d}}(x, D_i x, a_i) + 2T^x_{F^{[2]}_{2,d}}(x, D_i a_i) \\
&\quad + 2T^x_{F^{[3]}_{2,d}}(x, a_i, D_i x) + 2T^x_{F^{[3]}_{2,d}}(a_i, x, D_i x) + T^x_{F^{[2]}_{2,d}}(a_i, a_i).
\end{aligned}$$

Inserting both results into (8.1) yields Corollary 3.6. □

8.1. Conjugation property

The goal of this subsection is to show that I_2 satisfies the conjugation property of Proposition 8.5, which is needed in the proof of Theorem 3.8.

Firstly, we define a right action of $C^\infty(\mathbb{T}^d_\theta)$ on $\mathcal{X}$ by extending

$$\mathbf{D}_i b := D_i b + b\mathbf{D}_i \qquad (b \in C^\infty(\mathbb{T}^d_\theta)), \tag{8.3}$$

to a $C^\infty(\mathbb{T}^d_\theta)$-bimodule structure on $\mathcal{X}$ in the obvious way. (To be precise, $b\mathbf{D}^\alpha c = \sum_{\beta+\gamma=\alpha} bD^\beta c\mathbf{D}^\gamma$ if $\alpha \in \{0,1\}^d$, which one can assume without loss of generality.) One easily checks well-definedness of this structure. Moreover, using the notation introduced in (5.1), one easily checks that

$$\pi(b\mathbf{D}^\alpha c) = \lambda_l(b) D^\alpha \lambda_l(c), \tag{8.4}$$

for all $b, c \in C^\infty(\mathbb{T}^d_\theta)$ and $\alpha \in \mathbb{Z}^d_+$.

Lemma 8.2. *Let $x, y \in C^\infty(\mathbb{T}^d_\theta)$ with x self-adjoint, y invertible, and $[x, y] = 0$. We have*

$$\mathbf{T}^{x,2}_{F_{2,d}}(y^{-1}x\mathbf{D}_i y, y^{-1}x\mathbf{D}_i y) = y^{-1}\mathbf{T}^{x,2}_{F_{2,d}}(x\mathbf{D}_i, x\mathbf{D}_i)y + \frac{1}{2}y^{-1} \cdot x^2 F''_{2,d}(x) \cdot D_i^2 y$$
$$+ y^{-1}\Big(\mathbf{T}^{x,2}_{F_{2,d}}(x\mathbf{D}_i, x) + \mathbf{T}^{x,2}_{F_{2,d}}(x, x\mathbf{D}_i)\Big) \cdot D_i y.$$

Proof. Using (8.4) in the definition of $S^2_{s,z}$ (i.e., (5.2)), it follows that

$$S^2_{s,z}(y^{-1}x\mathbf{D}_i y, y^{-1}x\mathbf{D}_i y) = y^{-1}S^2_{s,z}(x\mathbf{D}_i, x\mathbf{D}_i y).$$

Again using the definition of $S^2_{s,z}$, we find

$$S^2_{s,z}(x\mathbf{D}_i, x\mathbf{D}_i y) = \frac{|s|^4 x}{x|s|^2 + z} D_i\Big(\frac{x}{x|s|^2 + z} D_i \frac{y}{x|s|^2 + z}\Big).$$

By the Leibniz rule, we have

$$\begin{aligned}
&D_i\Big(\frac{x}{x|s|^2 + z} D_i \frac{y}{x|s|^2 + z}\Big)\\
&\quad = D_i\Big(\frac{x}{(x|s|^2 + z)^2} \cdot D_i y\Big) + D_i\Big(\frac{x}{x|s|^2 + z} D_i\Big(\frac{1}{x|s|^2 + z}\Big) y\Big)\\
&\quad = \frac{x}{(x|s|^2 + z)^2} \cdot D_i^2 y + D_i\Big(\frac{x}{(x|s|^2 + z)^2}\Big) \cdot D_i y +\\
&\qquad + \frac{x}{x|s|^2 + z} D_i\Big(\frac{1}{x|s|^2 + z}\Big) \cdot D_i y + D_i\Big(\frac{x}{x|s|^2 + z} D_i\Big(\frac{1}{x|s|^2 + z}\Big)\Big) \cdot y.
\end{aligned}$$

Again appealing to the definition (5.2) of $S^2_{s,z}$, we write

$$\begin{aligned}
&S^2_{s,z}(x\mathbf{D}_i, x\mathbf{D}_i y)\\
&\quad = S^2_{s,z}(x, x)D_i^2 y + S^2_{s,z}(x\mathbf{D}_i, x)D_i y + S^2_{s,z}(x, x\mathbf{D}_i)D_i y + S^2_{s,z}(x\mathbf{D}_i, x\mathbf{D}_i)y.
\end{aligned}$$

By doubly integrating both sides of the above equality, applying Corollary 7.1 to the resulting terms, and using that

$$T^x_{F^{[2]}_{2,d}}(x, x) = x^2 \frac{1}{2} F''_{2,d}(x),$$

the lemma follows. □

Lemma 8.3. *Let $x, y \in C^\infty(\mathbb{T}^d_\theta)$ be invertible with $x \geq 0$ and $[x, y] = 0$. We have*

$$\mathbf{T}^{x,1}_{F_{2,d}}(y^{-1}x\mathbf{\Delta} y) = y^{-1}xF'_{2,d}(x)\Delta y + 2\sum_{i=1}^d y^{-1}\mathbf{T}^{x,1}_{F_{2,d}}(x\mathbf{D}_i)D_i y + y^{-1}\mathbf{T}^{x,1}_{F_{2,d}}(x\mathbf{\Delta})y.$$

Proof. By using (8.4) in the definition of $S^1_{s,z}$, we find

$$S^1_{s,z}(y^{-1}x\mathbf{\Delta}y) = -\frac{|s|^2y^{-1}x}{x|s|^2+z}\Delta\Big(\frac{y}{x|s|^2+z}\Big).$$

By the Leibniz rule, we have

$$\Delta\Big(\frac{y}{x|s|^2+z}\Big) = \frac{1}{x|s|^2+z}\Delta y + 2\sum_{i=1}^d D_i\Big(\frac{1}{x|s|^2+z}\Big)\cdot D_i y + \Delta\Big(\frac{1}{x|s|^2+z}\Big)\cdot y.$$

Thus,

$$S^1_{s,z}(y^{-1}x\mathbf{\Delta}y) = y^{-1}S^1_{s,z}(x)\Delta y + 2\sum_{i=1}^d y^{-1}S^1_{s,z}(x\mathbf{D}_i)D_i y + y^{-1}S^1_{s,z}(x\mathbf{\Delta})y.$$

Like in the previous proof, the assertion follows by appealing to Corollary 7.1. □

Lemma 8.4. *Let $x \in C^\infty(\mathbb{T}^d_\theta)$ be positive and invertible. We have*

$$d\mathbf{T}^{x,1}_{F_{2,d}}(x\mathbf{D}_i) + 2\mathbf{T}^{x,2}_{F_{2,d}}(x\mathbf{D}_i, x) + 2\mathbf{T}^{x,2}_{F_{2,d}}(x, x\mathbf{D}_i) = 0. \tag{8.5}$$

Proof. By the recursive definition of $\mathbf{T}^{x,m}_\phi$ (Definition 3.1), we have

$$d\mathbf{T}^{x,1}_{F_{2,d}}(x\mathbf{D}_i) = dT^x_{F^{[2]}_{2,d}}(x, D_i x), \quad 2\mathbf{T}^{x,2}_{F_{2,d}}(x, x\mathbf{D}_i) = 2T^x_{F^{[3]}_{2,d}}(x, x, D_i x), \tag{8.6}$$

$$\begin{aligned} 2\mathbf{T}^{x,2}_{F_{2,d}}(x\mathbf{D}_i, x) &= 2\mathbf{T}^{x,3}_{F_{2,d}}(x, D_i x, x) + 2\mathbf{T}^{x,2}_{F_{2,d}}(x, D_i x) + 2\mathbf{T}^{x,2}_{F_{2,d}}(x, x\mathbf{D}_i) \\ &= 2T^x_{F^{[3]}_{2,d}}(x, D_i x, x) + 2T^x_{F^{[2]}_{2,d}}(x, D_i x) + 2T^x_{F^{[3]}_{2,d}}(x, x, D_i x). \end{aligned} \tag{8.7}$$

By the definition of the multiple operator integral, we may rewrite the above terms as $T_\phi(D_i x)$, for instance, for any function f we may rewrite

$$T^x_f(x, D_i x, x) = T^x_{\phi_1}(D_i x), \qquad \text{where} \qquad \phi_1(\alpha_0, \alpha_1) = \alpha_0 f(\alpha_0, \alpha_0, \alpha_1, \alpha_1)\alpha_1.$$

In the same way, by using (8.6) and (8.7), the left-hand side of (8.5) equals $T^x_\phi(D_i x)$, where

$$\begin{aligned} \phi(\alpha_0, \alpha_1) =& d\alpha_0 F^{[2]}_{2,d}(\alpha_0, \alpha_0, \alpha_1) + 2\alpha_0\alpha_1 F^{[3]}_{2,d}(\alpha_0, \alpha_0, \alpha_1, \alpha_1) \\ &+ 2\alpha_0 F^{[2]}_{2,d}(\alpha_0, \alpha_0, \alpha_1) + 4\alpha_0^2 F^{[3]}_{2,d}(\alpha_0, \alpha_0, \alpha_0, \alpha_1). \end{aligned}$$

Note that ϕ is homogeneous. Thus, it suffices to prove that $\phi(1, \alpha) = 0$. In other words, we need to show

$$(d+2)F^{[2]}_{2,d}(1, 1, \alpha) + 2\alpha F^{[3]}_{2,d}(1, 1, \alpha, \alpha) + 4F^{[3]}_{2,d}(1, 1, 1, \alpha) = 0.$$

This equality is an elementary exercise, albeit rather long, and its proof is omitted. □

Proposition 8.5. *Let $x, y \in C^\infty(\mathbb{T}^d_\theta)$ be invertible with $x \geq 0$ and $[x, y] = 0$. We have*

$$I_2(\lambda_l(y^{-1}x)\Delta\lambda_l(y)) = y^{-1} \cdot I_2(\lambda_l(x)\Delta) \cdot y.$$

Proof. From (8.3) we obtain

$$y^{-1}x\mathbf{\Delta}y = x\mathbf{\Delta} + \sum_{i=1}^{d} a_i\mathbf{D}_i + a,$$
$$a_i = 2y^{-1}xD_i(y), \quad 1 \leq i \leq d, \quad a = y^{-1}x\Delta y.$$

From this one can derive that

$$\mathbf{A}_i = 2y^{-1}x\mathbf{D}_iy.$$

By Lemma 8.1 we have

$$-\pi^{-\frac{d}{2}}I_2(\lambda_l(y^{-1}x)\Delta\lambda_l(y)) = \mathbf{T}^{x,1}_{F_{2,d}}(y^{-1}x\mathbf{\Delta}y) + \frac{4}{d}\sum_{i=1}^{d}\mathbf{T}^{x,2}_{F_{2,d}}(y^{-1}x\mathbf{D}_iy, y^{-1}x\mathbf{D}_iy).$$

Using Lemma 8.2 and Lemma 8.3, we write

$$\begin{aligned}
&-\pi^{-\frac{d}{2}}I_2(\lambda_l(y^{-1}x)\Delta\lambda_l(y)) \\
=&y^{-1}\Big(\mathbf{T}^{x,1}_{F_{2,d}}(x\mathbf{\Delta}) + \frac{4}{d}\sum_{i=1}^{d}\mathbf{T}^{x,2}_{F_{2,d}}(x\mathbf{D}_i, x\mathbf{D}_i)\Big) + y^{-1}\Big(xF'_{2,d}(x) + \frac{2}{d}x^2F''_{2,d}(x)\Big)\Delta y+ \\
&+\sum_{i=1}^{d}y^{-1}\Big(2\mathbf{T}^{x,1}_{F_{2,d}}(x\mathbf{D}_i) + \frac{4}{d}\mathbf{T}^{x,2}_{F_{2,d}}(x\mathbf{D}_i, x) + \frac{4}{d}\mathbf{T}^{x,2}_{F_{2,d}}(x, x\mathbf{D}_i)\Big)D_iy.
\end{aligned}$$

Since $F_{2,d}$ is the primitive of $\alpha \to \alpha^{-\frac{d}{2}}$, it follows that

$$xF'_{2,d}(x) + \frac{2}{d}x^2F''_{2,d}(x) = x \cdot x^{-\frac{d}{2}} + \frac{2x^2}{d} \cdot (-\frac{d}{2}x^{-1-\frac{d}{2}}) = 0.$$

So, the second summand on the right hand side vanishes. Third summand on the right hand side vanishes by Lemma 8.4. This completes the proof. □

8.2. Proof of Theorem 3.8

Lemma 8.6. *Let $x \in C^\infty(\mathbb{T}^d_\theta)$ be positive and invertible. Let $d \geq 2$. We have*

$$-\pi^{-\frac{d}{2}}I_2(\lambda_l(x^{\frac{1}{2}})\Delta\lambda_l(x^{\frac{1}{2}})) = T^x_\Phi(\Delta x) + \sum_{i=1}^{d}T^x_\Psi(D_ix, D_ix),$$

for the symbols Φ, Ψ *defined by* $F_{2,d}$*, a first order primitive of* $\alpha \mapsto \alpha^{-\frac{d}{2}}$*, as*

$$\Phi(\alpha_0,\alpha_1) := \Big(\frac{\alpha_1}{\alpha_0}\Big)^{\frac{1}{2}}\Big(\alpha_0 F_{2,d}^{[2]}(\alpha_0,\alpha_0,\alpha_1) + \frac{4}{d}\alpha_0^2 F_{2,d}^{[3]}(\alpha_0,\alpha_0,\alpha_0,\alpha_1)\Big),$$

$$\begin{aligned}\Psi(\alpha_0,\alpha_1,\alpha_2) :=& (\frac{\alpha_2}{\alpha_0})^{\frac{1}{2}}\Big(\frac{4}{d}\alpha_0\alpha_1 F_{2,d}^{[4]}(\alpha_0,\alpha_0,\alpha_1,\alpha_1,\alpha_2)\\ &+ (2+\frac{4}{d})\alpha_0 F_{2,d}^{[3]}(\alpha_0,\alpha_0,\alpha_1,\alpha_2) + \frac{8}{d}\alpha_0^2 F_{2,d}^{[4]}(\alpha_0,\alpha_0,\alpha_0,\alpha_1,\alpha_2)\Big),\end{aligned}$$

for $\alpha_0,\alpha_1,\alpha_2,\alpha > 0$.

Proof. Using Corollary 3.6 we find

$$\begin{aligned}-\pi^{-\frac{d}{2}} I_2(\lambda_l(x)\Delta) =& T^x_{F_{2,d}^{[2]}}(x,\Delta x) + \frac{4}{d}T^x_{F_{2,d}^{[3]}}(x,x,\Delta x) + \sum_{i=1}^{2}\Big(\frac{4}{d}T^x_{F_{2,d}^{[4]}}(x,D_i x,x,D_i x)\\ &+ (2+\frac{4}{d})T^x_{F_{2,d}^{[3]}}(x,D_i x,D_i x) + \frac{8}{d}T^x_{F_{2,d}^{[4]}}(x,x,D_i x,D_i x)\Big).\end{aligned}$$

Combining the above formula with Proposition 8.5 and computing the resulting symbols yields the lemma. □

The rest of this section consists purely of algebraically rewriting the above formulas for Φ and Ψ into a more concise form, and thusly derives Theorem 3.8. Let us again fix $d \geq 2$ and $F_{2,d}$ as in Remark 3.4.

Lemma 8.7. *For* Φ *as in Lemma 8.6, we have*

$$\Phi(\alpha_0,\alpha_1) = \frac{2(\alpha_0\alpha_1)^{\frac{1}{2}}}{d}\cdot\frac{\alpha_0 F_{2,d}^{[2]}(\alpha_0,\alpha_0,\alpha_1) - \alpha_1 F_{2,d}^{[2]}(\alpha_0,\alpha_1,\alpha_1)}{\alpha_1-\alpha_0}, \quad \alpha_0,\alpha_1 > 0.$$

Proof. By definition of Φ in Lemma 8.6, we have ($\alpha_0,\alpha_1 > 0$ as always)

$$(\alpha_0\alpha_1)^{-\frac{1}{2}}\Phi(\alpha_0,\alpha_1) = F_{2,d}^{[2]}(\alpha_0,\alpha_0,\alpha_1) + \frac{4}{d}\alpha_0 F_{2,d}^{[3]}(\alpha_0,\alpha_0,\alpha_0,\alpha_1).$$

Thus,

$$\begin{aligned}&(\alpha_1-\alpha_0)\cdot(\alpha_0\alpha_1)^{-\frac{1}{2}}\Phi(\alpha_0,\alpha_1)\\ &= F_{2,d}^{[1]}(\alpha_0,\alpha_1) - F_{2,d}^{[1]}(\alpha_0,\alpha_0) + \frac{4\alpha_0}{d}F_{2,d}^{[2]}(\alpha_0,\alpha_0,\alpha_1) - \frac{4\alpha_0}{d}F_{2,d}^{[2]}(\alpha_0,\alpha_0,\alpha_0).\end{aligned}$$

By definition,

$$F_{2,d}^{[1]}(\alpha_0,\alpha_0) + \frac{4\alpha_0}{d}F_{2,d}^{[2]}(\alpha_0,\alpha_0,\alpha_0) = F'_{2,d}(\alpha_0) + \frac{2\alpha_0}{d}F''_{2,d}(\alpha_0) = 0.$$

Thus,

$$(\alpha_1-\alpha_0)\cdot(\alpha_0\alpha_1)^{-\frac{1}{2}}\Phi(\alpha_0,\alpha_1)=F_{2,d}^{[1]}(\alpha_0,\alpha_1)+\frac{4\alpha_0}{d}F_{2,d}^{[2]}(\alpha_0,\alpha_0,\alpha_1)$$

and

$$\begin{aligned}&(\alpha_1-\alpha_0)^2\cdot(\alpha_0\alpha_1)^{-\frac{1}{2}}\Phi(\alpha_0,\alpha_1)\\&=F_{2,d}(\alpha_1)-F_{2,d}(\alpha_0)+\frac{4\alpha_0}{d}F_{2,d}^{[1]}(\alpha_0,\alpha_1)-\frac{4\alpha_0}{d}F_{2,d}^{[1]}(\alpha_0,\alpha_0)\\&=(1-\frac{2}{d})\big(F_{2,d}(\alpha_1)-F_{2,d}(\alpha_0)\big)+\frac{2(\alpha_0+\alpha_1)}{d}F_{2,d}^{[1]}(\alpha_0,\alpha_1)-\frac{4\alpha_0}{d}F_{2,d}'(\alpha_0).\end{aligned}$$

The right-hand side, clearly, equals

$$\begin{aligned}&\frac{2}{d}\Big((\alpha_0+\alpha_1)F_{2,d}^{[1]}(\alpha_0,\alpha_1)-(\alpha_0^{1-\frac{d}{2}}+\alpha_1^{1-\frac{d}{2}})\Big)\\&=\frac{2}{d}\Big(\alpha_0(F_{2,d}^{[1]}(\alpha_0,\alpha_1)-F_{2,d}'(\alpha_0))+\alpha_1(F_{2,d}^{[1]}(\alpha_0,\alpha_1)-F_{2,d}'(\alpha_1))\Big)\\&=\frac{2}{d}\Big(\alpha_0(\alpha_1-\alpha_0)F_{2,d}^{[2]}(\alpha_0,\alpha_0,\alpha_1)-\alpha_1(\alpha_1-\alpha_0)F_{2,d}^{[2]}(\alpha_0,\alpha_1,\alpha_1)\Big).\end{aligned}$$

Thus,

$$(\alpha_1-\alpha_0)\cdot(\alpha_0\alpha_1)^{-\frac{1}{2}}\Phi(\alpha_0,\alpha_1)=\frac{2}{d}\Big(\alpha_0F_{2,d}^{[2]}(\alpha_0,\alpha_0,\alpha_1)-\alpha_1F_{2,d}^{[2]}(\alpha_0,\alpha_1,\alpha_1)\Big).\quad\square$$

Lemma 8.8. *Let $f,g\in C^\infty((0,\infty))$ be such that $f+g'=0$. If*

$$\psi(\alpha,\beta)=f^{[2]}(\alpha,\alpha,\beta)+2g^{[3]}(\alpha,\alpha,\alpha,\beta),$$

then

$$\psi(\alpha,\beta)=-g^{[3]}(\alpha,\alpha,\beta,\beta).$$

Proof. As $f=-g'$, we have

$$\begin{aligned}\psi(\alpha,\beta)&=-(g')^{[2]}(\alpha,\alpha,\beta)+2g^{[3]}(\alpha,\alpha,\alpha,\beta)\\&=-\frac{(g')^{[1]}(\alpha,\beta)-(g')^{[1]}(\alpha,\alpha)}{\beta-\alpha}+2\frac{g^{[2]}(\alpha,\alpha,\beta)-\frac{1}{2}g^{(2)}(\alpha)}{\beta-\alpha}\\&=\frac{1}{\beta-\alpha}\Big(2g^{[2]}(\alpha,\alpha,\beta)-(g')^{[1]}(\alpha,\beta)\Big)\\&=\frac{1}{\beta-\alpha}\Big(2\frac{g^{[1]}(\alpha,\alpha)-g^{[1]}(\alpha,\beta)}{\alpha-\beta}-\frac{g^{[1]}(\alpha,\alpha)-g^{[1]}(\beta,\beta)}{\alpha-\beta}\Big)\end{aligned}$$

$$= \frac{1}{\beta-\alpha}\Big(\frac{g^{[1]}(\alpha,\alpha)-g^{[1]}(\alpha,\beta)}{\alpha-\beta} - \frac{g^{[1]}(\alpha,\beta)-g^{[1]}(\beta,\beta)}{\alpha-\beta}\Big)$$

$$= \frac{1}{\beta-\alpha}(g^{[2]}(\alpha,\alpha,\beta)-g^{[2]}(\alpha,\beta,\beta)),$$

concluding the proof. □

Lemma 8.9. *For* Ψ *as in Lemma 8.6, we have*

$$\Psi(\alpha,1,\beta) = -\frac{4}{d}(\alpha\beta)^{\frac{1}{2}}g^{[3]}(\alpha,\alpha,\beta,\beta), \quad \alpha,\beta>0.$$

Here,

$$g(\alpha) = F_{2,d}(\alpha) + F_{2,d}^{[1]}(1,\alpha), \quad \alpha>0.$$

Proof. By definition of Ψ in Lemma 8.6, we have

$$\frac{d}{4}\frac{1}{(\alpha\beta)^{\frac{1}{2}}}\Psi(\alpha,1,\beta)$$
$$= F_{2,d}^{[4]}(\alpha,\alpha,1,1,\beta) + \Big(\frac{d}{2}+1\Big)F_{2,d}^{[3]}(\alpha,\alpha,1,\beta) + 2\alpha F_{2,d}^{[4]}(\alpha,\alpha,\alpha,1,\beta).$$

Note that

$$\alpha F_{2,d}^{[4]}(\alpha,\alpha,\alpha,1,\beta) = (\alpha-1)F_{2,d}^{[4]}(\alpha,\alpha,\alpha,1,\beta) + F_{2,d}^{[4]}(\alpha,\alpha,\alpha,1,\beta)$$
$$= F_{2,d}^{[3]}(\alpha,\alpha,\alpha,\beta) - F_{2,d}^{[3]}(\alpha,\alpha,1,\beta) + F_{2,d}^{[4]}(\alpha,\alpha,\alpha,1,\beta).$$

Thus,

$$\frac{d}{4}\frac{1}{(\alpha\beta)^{\frac{1}{2}}}\Psi(\alpha,1,\beta) = F_{2,d}^{[4]}(\alpha,\alpha,1,1,\beta) + \Big(\frac{d}{2}-1\Big)F_{2,d}^{[3]}(\alpha,\alpha,1,\beta)$$
$$+ 2F_{2,d}^{[3]}(\alpha,\alpha,\alpha,\beta) + 2F_{2,d}^{[4]}(\alpha,\alpha,\alpha,1,\beta)$$
$$= f^{[2]}(\alpha,\alpha,\beta) + 2g^{[3]}(\alpha,\alpha,\alpha,\beta),$$

where

$$f(\alpha) = F_{2,d}^{[2]}(1,1,\alpha) + \Big(\frac{d}{2}-1\Big)F_{2,d}^{[1]}(1,\alpha); \qquad g(\alpha) = F_{2,d}(\alpha) + F_{2,d}^{[1]}(1,\alpha).$$

By writing out the divided differences explicitly, it is straightforward to show that $f+g' = 0$. The assertion now follows from Lemma 8.8. □

Proof of Theorem 3.8. By Lemma 8.6, we obtain the assertion of Theorem 3.8, with alternate expressions for Φ and Ψ. It is established in Lemma 8.7 that the expressions for Φ in Lemma 8.6 and in Theorem 3.8 coincide.

Note that Ψ (as in Lemma 8.6) is homogeneous of degree $-1-\frac{d}{2}$, so that

$$\Psi(\alpha_0,\alpha_1,\alpha_2)=\alpha_1^{-1-\frac{d}{2}}\Psi(\frac{\alpha_0}{\alpha_1},1,\frac{\alpha_2}{\alpha_1}),\quad \alpha_0,\alpha_1,\alpha_2>0.$$

The required convenient expression for Ψ now follows from Lemma 8.9. □

9. Recovering the Connes–Moscovici modular curvature

In [7], and, independently, in [13], a formula for the so-called scalar curvature $I_2(P)$ of the conformally deformed non-commutative two-torus is given in terms of the modular operator of the corresponding conformal factors. Below we show how to recover their formulas as a special case of our result by taking $P=\lambda_l(x^{1/2})\Delta\lambda_l(x^{1/2})$, which in the notation of [7] and [13] corresponds to the Laplacian on functions when $\tau=i$.

For our convenience, we define the modular functional calculus as follows.

Definition 9.1. Let $d\in\mathbb{N}_{\geq 2}$, $n\in\mathbb{N}$, and $x,V_1,\dots,V_n\in L_\infty(\mathbb{T}^d_\theta)$ with x positive and invertible. For any $K\in C^\infty(\mathbb{R})$, $H\in C^\infty(\mathbb{R}^2)$, and $L\in C^\infty(\mathbb{R}^n)$, we set

$$K(\nabla)(V_1):=T^x_{K(\log(\frac{\alpha_1}{\alpha_0}))}(V_1),\quad H(\nabla_1,\nabla_2)(V_1,V_2):=T^x_{H(\log(\frac{\alpha_1}{\alpha_0}),\log(\frac{\alpha_2}{\alpha_1}))}(V_1,V_2),$$
$$L(\nabla_1,\dots,\nabla_n)(V_1,\dots,V_n):=T^x_{L(\log(\alpha_1/\alpha_0),\dots,\log(\alpha_n/\alpha_{n-1}))}(V_1,\dots,V_n).$$

Here and in the following, a multiple operator integral $T^x_{f(\alpha_0,\dots,\alpha_n)}$ should be understood as $T^x_{(\alpha_0,\dots,\alpha_n)\mapsto f(\alpha_0,\dots,\alpha_n)}$.

Consider as an important example the case that $K(\log(\alpha))=\alpha^p$. Then

$$T^x_{K(\log(\frac{\alpha_1}{\alpha_0}))}(V_1)=T^x_{\alpha_0^{-p}\alpha_1^p}(V_1)=x^{-p}V_1x^p=\tilde{\Delta}^p(V_1)=K(\log\tilde{\Delta})(V_1),$$

where $\tilde{\Delta}:V_1\mapsto e^{-h}V_1e^h$ is the modular operator corresponding to the conformal factor $h=\log x$. Extending this argument a bit further, one finds that the above definition agrees with the definitions of [7,13]; see [28] for more clarification.

Lemma 9.2. *Let $d\in\mathbb{N}_{\geq 2}$. If $x=e^h$ for self-adjoint $h\in C^\infty(\mathbb{T}^d_\theta)$ then for all $K\in C^\infty(\mathbb{R})$ and $H\in C^\infty(\mathbb{R}^2)$ we have*

$$T^x_{\Phi_K}(\Delta x)+\sum_{i=1}^d T^x_{\Psi_{K,H}}(D_ix,D_ix)=\frac{1}{2}K(\nabla)(\Delta h)+\frac{1}{4}\sum_{i=1}^d H(\nabla_1,\nabla_2)(D_ih,D_ih),$$

for

$$\Phi_K(\alpha_0,\alpha_1) = \frac{1}{2}K(\log(\frac{\alpha_1}{\alpha_0}))\cdot\log^{[1]}(\alpha_0,\alpha_1);$$

$$\Psi_{K,H}(\alpha_0,\alpha_1,\alpha_2) = K(\log(\frac{\alpha_2}{\alpha_0}))\cdot\log^{[2]}(\alpha_0,\alpha_1,\alpha_2) + \frac{1}{4}H(\log(\frac{\alpha_1}{\alpha_0}),\log(\frac{\alpha_2}{\alpha_1}))\cdot\log^{[1]}(\alpha_0,\alpha_1)\cdot\log^{[1]}(\alpha_1,\alpha_2).$$

Proof. As $C^\infty(\mathbb{T}^d_\theta)$ is stable under holomorphic functional calculus, we have $x = e^h \in C^\infty(\mathbb{T}^d_\theta)$. By standard arguments in multiple operator integration theory, we find

$$D_i h = T^x_{\log^{[1]}}(D_i x);\quad \Delta h = T^x_{\log^{[1]}}(\Delta x) + 2\sum_{i=1}^d T^x_{\log^{[2]}}(D_i x, D_i x).$$

Applying Definition 9.1, we obtain the lemma. □

It turns out that $\Phi_{K_0} = \Phi$ and $\Psi_{K_0,H_0} = \Psi$ with Φ,Ψ as in Theorem 3.8 and K_0 and H_0 precisely as in the following theorem, proven in an entirely different way in [7].

Theorem 9.3 *(Connes–Moscovici). Let $x = e^h$ for self-adjoint $h \in C^\infty(\mathbb{T}^2_\theta)$ and consider $P = \lambda_l(x^{1/2})\Delta\lambda_l(x^{1/2})$ acting in $L_2(\mathbb{T}^2_\theta)$. We have*

$$I_2(P) = -\frac{\pi}{2}\left(K_0(\nabla)(\Delta h) + \frac{1}{2}\sum_{i=1}^2 H_0(\nabla_1,\nabla_2)(D_i h, D_i h)\right),$$

where

$$K_0(s) := \frac{-2+s\coth\left(\frac{s}{2}\right)}{s\sinh\left(\frac{s}{2}\right)};\qquad H_0(s,t) :=$$
$$\frac{t(s+t)\cosh(s) - s(s+t)\cosh(t) + (s-t)(s+t+\sinh(s)+\sinh(t)-\sinh(s+t))}{st(s+t)\sinh(s/2)\sinh(t/2)\sinh^2((s+t)/2)}.$$

Proof. Let Φ,Ψ be as in Theorem 3.8. A straightforward computation shows that

$$\Phi(1,\alpha) = \frac{1}{2}K_0(\log(\alpha))\cdot\frac{\log(\alpha)}{\alpha-1},$$

for $\alpha > 0$. By homogeneity, this yields

$$\Phi(\alpha_0,\alpha_1) = \frac{1}{2}K_0(\log(\frac{\alpha_1}{\alpha_0}))\log^{[1]}(\alpha_0,\alpha_1) = \Phi_{K_0}(\alpha_0,\alpha_1),\quad \alpha_0,\alpha_1 > 0,$$

with Φ_{K_0} as in Lemma 9.2.

We are now left to show that $\Psi = \Psi_{K_0,H_0}$, which by homogeneity comes down to showing that

$$
\begin{aligned}
-2(\alpha\beta)^{\frac{1}{2}} g^{[3]}(\alpha,\alpha,\beta,\beta) =& K_0(\log(\beta/\alpha))\cdot \log^{[2]}(\alpha,1,\beta)\\
&+\frac{1}{4}H_0(-\log(\alpha),\log(\beta))\cdot \log^{[1]}(\alpha,1)\cdot \log^{[1]}(1,\beta).
\end{aligned}
$$

By writing $-\log(\alpha) = s$ and $\log(\beta) = t$, one finds

$$
\begin{aligned}
&\frac{4}{\log^{[1]}(\alpha,1)\log^{[1]}(1,\beta)}\left(-2(\alpha\beta)^{\frac{1}{2}} g^{[3]}(\alpha,\alpha,\beta,\beta) - K_0(\log(\beta/\alpha))\cdot \log^{[2]}(\alpha,1,\beta)\right)\\
&= \frac{4}{\frac{(-st)}{(e^{-s}-1)(e^{t}-1)}}\Bigg(-2e^{-\frac{s}{2}}e^{\frac{t}{2}}\frac{1}{(e^{-s}-e^{t})^2}\Bigg(\frac{s}{(e^{-s}-1)^2}+\frac{1}{e^{-s}-1}\\
&\quad -\frac{2}{e^{-s}-e^{t}}\left(\frac{e^{-s}}{e^{-s}-1}(-s)-\frac{e^{t}}{e^{t}-1}t\right)+\frac{-t}{(e^{t}-1)^2}+\frac{1}{e^{t}-1}\Bigg)\\
&\quad -\left(-\frac{4e^{\frac{(t+s)}{2}}}{(t+s)\left(e^{(t+s)}-1\right)}+2e^{\left(\frac{t+s}{2}\right)}\left(\frac{\left(e^{(t+s)}+1\right)}{\left(e^{(t+s)}-1\right)^2}\right)\right)\\
&\quad \cdot\left(\frac{1}{e^{-s}-e^{t}}\left(-\frac{s}{e^{-s}-1}-\frac{t}{e^{t}-1}\right)\right)\Bigg).
\end{aligned}
$$

Upon multiplying the latter expression with the denominator of $H_0(s,t)$, i.e.,

$$
st(s+t)\sinh(s/2)\sinh(t/2)\sinh^2((s+t)/2),
$$

and writing the result out explicitly, one straightforwardly obtains the numerator of $H_0(s,t)$, i.e.,

$$
t(s+t)\cosh(s) - s(s+t)\cosh(t) + (s-t)(s+t+\sinh(s)+\sinh(t)-\sinh(s+t)).
$$

This concludes the proof. □

9.1. K_0 for general d

We now give an example of a completely new modular formula that can be obtained from our main result, which generalises the function K_0 that appears in the main result of [7] to any dimension.

Theorem 9.4. *For all $d \in \mathbb{N}_{\geq 3}$, $x = e^h$, $h = h^* \in C^\infty(\mathbb{T}^d_\theta)$, $P = \lambda_l(x^{1/2})\Delta\lambda_l(x^{1/2})$ acting in $L_2(\mathbb{T}^d_\theta)$, we have*

$$
I_2(P) = -\frac{\pi^{d/2}}{2}e^{(1-d/2)h}\left(K_0^d(\nabla)(\Delta h) + \frac{1}{2}\sum_{i=1}^{d} H_0^d(\nabla_1,\nabla_2)(D_i h, D_i h)\right), \quad (9.1)
$$

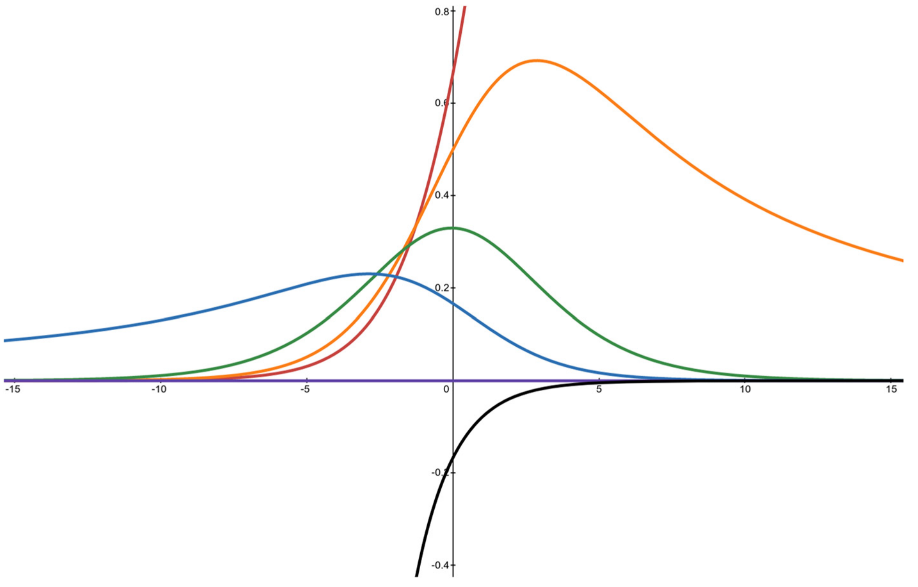

Fig. 1. The function K_0^d for $d = 0.01$ (red), $d = 1$ (orange), $d = 2.01$ (green), $d = 3$ (blue), $d = 4$ (purple, horizontal axis), and $d = 5$ (black), plotted with Desmos. (For interpretation of the colours in the figure(s), the reader is referred to the web version of this article.)

for some function H_0^d *and*

$$K_0^d(s) = \frac{2}{d} \cdot \frac{-1 - e^{(1-\frac{d}{2})s} + \frac{e^{(1-d/2)s}-1}{1-d/2}\coth\left(\frac{s}{2}\right)}{s\sinh\left(\frac{s}{2}\right)}. \tag{9.2}$$

The above formula in fact defines a function K_0^d *for every* $d \in (2, \infty)$, *satisfying*

$$\lim_{d\to 2} K_0^d(s) = K_0(s),$$

with K_0 *as in Theorem 9.3. Moreover,* $K_0^4 = 0$ *(see Fig. 1).*

Proof. By Theorem 3.8 and Lemma 9.2, we obtain (9.1) exactly when $\Phi(\alpha_0, \alpha_1) = \alpha_0^{1-\frac{d}{2}} \Phi_{K_0^d}(\alpha_0, \alpha_1)$ and $\Psi(\alpha_0, \alpha_1, \alpha_2) = \alpha_0^{1-\frac{d}{2}} \Psi_{K_0^d, H_0^d}(\alpha_0, \alpha_1, \alpha_2)$. By homogeneity, we are left to derive (9.2) for the function K_0^d defined by

$$K_0^d(\log(\alpha)) := \frac{2}{\log^{[1]}(1, \alpha)} \cdot \Phi(1, \alpha), \tag{9.3}$$

with Φ from Theorem 3.8, namely

$$\Phi(1, \alpha) = \frac{2\alpha^{1/2}}{d} \frac{F_{2,d}^{[2]}(1, 1, \alpha) - \alpha F_{2,d}^{[2]}(1, \alpha, \alpha)}{\alpha - 1}. \tag{9.4}$$

Combining (9.3) with (9.4) and substituting $\alpha = e^s$, we obtain

$$K_0^d(s) = \frac{2(e^s-1)}{s} \cdot \frac{2e^{s/2}}{d} \left(\frac{1}{(e^s-1)^2} \left(\frac{1}{1-\frac{d}{2}} \frac{e^{(1-\frac{d}{2})s}-1}{e^s-1} - 1 \right) - \frac{e^s}{(e^s-1)^2} \left(e^{-\frac{d}{2}s} - \frac{1}{1-\frac{d}{2}} \frac{e^{(1-\frac{d}{2})s}-1}{e^s-1} \right) \right).$$

Simplifying the above formula, one obtains the desired form of K_0^d. The last two statements of the theorem follow by using $\lim_{d\to 2} \frac{e^{(1-d/2)s}-1}{1-d/2} = s$ and $\coth(\frac{s}{2}) = \frac{1+e^{-s}}{1-e^{-s}}$, respectively. □

Generalisations of the functions H_0, K, H, S *et cetera* appearing in the main result [7, Theorem 3.2] can be similarly obtained. In fact, similar formulas for $k > 2$ are now within easy reach. Although we have proved the theorem above as a consequence of Theorem 3.8 (which we think is interesting in its own right) we stress that it can also be obtained directly from Theorem 3.3, with the only difference that the intermediate formulas become longer. In this way one can obtain any function in the modular operator, for any P and k one chooses.

10. The relation with the Iochum–Masson-approach for rational θ

We now relate our approach with the one of [24–26], in which Iochum and Masson calculate the local invariants for differential operators on finite dimensional bundles over manifolds. Suppose that $\theta \in M_d(\mathbb{R})$ is such that we can identify

$$C^\infty(\mathbb{T}^d_\theta) \subseteq M_N(C^\infty(\mathbb{T}^d)),$$

where $M_N(C^\infty(\mathbb{T}^d))$ is the algebra of $N \times N$ matrices with entries in $C^\infty(\mathbb{T}^d)$. There is such an inclusion for $d = 2$ and rational θ, or in higher dimensions under a slightly more convoluted condition on the entries of $\theta \in M_d(\mathbb{R})$ (cf. [38]). In these cases the results of [24–26] can be applied. In [25, Appendix B], the final result of [25] is compared to the final result of [13], for $k = 2$ and $d = 2$. Here, we compare our result to [24] for any d and any k.

For all $m \in \mathbb{N}$, $\xi \in \mathbb{R}^d$ and all matrix-valued differential operators $B_1, \dots, B_m$, [24, eq. (2.1)] defines a matrix denoted $f_m(\xi)[B_1 \otimes \cdots \otimes B_m] \in M_N(\mathbb{C})$, by setting, for all $v \in \mathbb{C}^N$,

$$f_m(\xi)[B_1 \otimes \cdots \otimes B_m]v := \int_{\Delta_m} e^{(s_1-1)|\xi|^2\lambda_l(x)} B_1 e^{(s_2-s_1)|\xi|^2\lambda_l(x)} \cdots B_m e^{(s_{m+1}-s_m)|\xi|^2\lambda_l(x)} (1_M \otimes v)\, ds, \tag{10.1}$$

where $(1_M \otimes v)$ is just the section in $C^\infty(\mathbb{T}^d;\mathbb{C}^N))$ that is constantly v, and $\Delta_m = \{s \in \mathbb{R}_+^m : \ 0 \leq s_m \leq \cdots \leq s_1 \leq 1\}$ is the simplex equipped with the flat measure ds of total variation $1/m!$, and $s_{m+1} := 0$. The integrand in (10.1) can be identified with a $\mathbb{C}^N$-valued function on $\mathbb{T}^d$ for every ξ and s, which for every ξ is Bochner-integrable in s.

With respect to the notation of [24], we restrict ourselves to $g^{\mu\nu} = \delta_{\mu\nu}$, and substitute $u^{\mu\nu} = x\delta_{\mu\nu}$, $v^\mu(\cdot) = ia_\mu$, $w = -a$, and $\mathrm{tr} = (2\pi)^d\tau$ into the formulas [24, eqs. (1.6-1.7)], and note that we may identify $-i\partial_j = D_j$. In this case, the formulas [24, (2.4-2.5), etc.] state that the local invariants of order $k \in \{0, 2, 4\}$ are given by

$$I_k(P) = \int_{\mathbb{R}^d} \sum_{\frac{k}{2} \leq m \leq k} (-1)^m \sum_{\substack{\mathscr{A} \subseteq \{1,\ldots,m\} \\ |\mathscr{A}| = 2m-k}} f_m(\xi)[W_1^{\mathscr{A}}(\xi) \otimes \cdots \otimes W_m^{\mathscr{A}}(\xi)]\, d\xi, \tag{10.2}$$

in which we use the notation $W_i^{\mathscr{A}}$ from (4.3). Clearly the formula (10.2) works for any k, which Iochum and Masson have also noted in personal communication.

We can express their 'functional calculus' (10.1) as a multiple operator integral.

Lemma 10.1. *For all elements $b_1 \ldots, b_m \in C^\infty(\mathbb{T}_\theta^d)$ we have*

$$(-1)^m f_m(\xi)[b_1 \otimes \cdots \otimes b_m] = T_{g^{[m]}}^{|\xi|^2 x}(b_1, \ldots, b_m), \tag{10.3}$$

where $g(\alpha) := e^{-\alpha}$.

Proof. We obtain,

$$\begin{aligned} &(-1)^m f_m(\xi)[b_1 \otimes \cdots \otimes b_m]v \\ &= (-1)^m \int_{\Delta_m} e^{(s_1-1)|\xi|^2 x} b_1 e^{(s_2-s_1)|\xi|^2 x} \cdots b_m e^{-s_m|\xi|^2 x} v\, ds. \end{aligned} \tag{10.4}$$

As $b_1, \ldots, b_m$ are bounded operators, the above expression is a multiple operator integral for which we can compute the symbol inductively. Indeed, by using

$$\frac{e^{-s_m\alpha_m} - e^{-s_m\alpha_{m+1}}}{\alpha_m - \alpha_{m+1}} = -\int_0^{s_m} e^{(s_{m+1}-s_m)\alpha_m} e^{-s_{m+1}\alpha_{m+1}}\, ds_{m+1}.$$

we find

$$(-1)^m \int_{\Delta_m} e^{(s_1-1)\alpha_0} e^{(s_2-s_1)\alpha_1} \cdots e^{-s_m\alpha_m}\, ds = g^{[m]}(\alpha_0, \ldots, \alpha_m),$$

which is the symbol of the multiple operator integral of (10.4). $\square$

Proposition 10.2. *For all* $b_1, \ldots, b_m \in C^\infty(\mathbb{T}^d_\theta)$ *we have*

$$\frac{1}{2\pi}|\xi|^{-2m} \int_{-\infty}^{\infty} S^m_{\xi,i\lambda}(b_1, \ldots, b_m) e^{i\lambda}\, d\lambda = (-1)^m f_m(\xi)[b_1 \otimes \cdots \otimes b_m]. \tag{10.5}$$

More generally, for all $\mathbf{B}_1, \ldots, \mathbf{B}_m \in \mathcal{X}$ *we have*

$$\frac{1}{2\pi}|\xi|^{-2m} \int_{-\infty}^{\infty} S^m_{\xi,i\lambda}(\mathbf{B}_1, \ldots, \mathbf{B}_m) e^{i\lambda}\, d\lambda = (-1)^m f_m(\xi)[\pi(\mathbf{B}_1) \otimes \cdots \otimes \pi(\mathbf{B}_m)].$$

Proof. By using change of variables in the definition of the multiple operator integral, and subsequently using Lemma 10.1, we obtain

$$\begin{aligned} |\xi|^{-2m} T^x_{(\sigma_{|\xi|^{-2}} g)^{[m]}}(b_1, \ldots, b_m) &= T^{|\xi|^2 x}_{g^{[m]}}(b_1, \ldots, b_m) \\ &= (-1)^m f_m(\xi)[b_1 \otimes \cdots \otimes b_m]. \end{aligned}$$

By applying (6.1) we find the first part of the proposition.

When replacing b_j in (10.5) by differential operators, the left-hand side satisfies the same recursive properties as the right-hand side: compare [24, Lemma 2.1] with our Lemma 5.1 and Lemma 5.2. By induction (in which (10.5) is the induction base) the second part of the proposition follows. □

Theorem 10.3. *Let* θ *be such that* $C(\mathbb{T}^d_\theta) \subseteq M_N(C(\mathbb{T}^d))$. *With the notations as above, we have, for all* $\frac{k}{2} \le m \le k$ *and* $\mathscr{A} \subseteq \{1, \ldots, d\}$ *with* $|\mathscr{A}| = 2m - k$,

$$\begin{aligned} &(-1)^{\frac{k}{2}} \pi^{\frac{d}{2}} \sum_{\iota:\mathscr{A}\to\{1,\ldots,d\}} c^{(\iota)}_d\, \mathbf{T}^{x,m}_{F_{k,d}}(\mathbf{W}^{\mathscr{A},\iota}_1, \ldots, \mathbf{W}^{\mathscr{A},\iota}_m) \\ &= \int_{\mathbb{R}^d} (-1)^m f_m(\xi)[W^{\mathscr{A}}_1(\xi) \otimes \cdots \otimes W^{\mathscr{A}}_m(\xi)]\, d\xi, \end{aligned} \tag{10.6}$$

and our main result (Theorem 3.3) therefore reproduces (10.2) *due to [24].*

Proof. By applying Corollary 7.1 and, subsequently, Proposition 10.2, we find

$$\begin{aligned} &(-1)^{\frac{k}{2}} \pi^{\frac{d}{2}} \sum_{\iota:\mathscr{A}\to\{1,\ldots,d\}} c^{(\iota)}_d\, \mathbf{T}^{x,m}_{F_{k,d}}(\mathbf{W}^{\mathscr{A},\iota}_1, \ldots, \mathbf{W}^{\mathscr{A},\iota}_m) \\ &= \sum_{\iota:\mathscr{A}\to\{1,\ldots,d\}} c^{(\iota)}_d \frac{1}{2\pi} \int_{\mathbb{R}^d} |\xi|^{-k} \int_{-\infty}^{\infty} S^m_{\xi,i\lambda}(\mathbf{W}^{\mathscr{A},\iota}_1, \ldots, \mathbf{W}^{\mathscr{A},\iota}_m) e^{i\lambda}\, d\lambda\, d\xi \\ &= (-1)^m \sum_{\iota:\mathscr{A}\to\{1,\ldots,d\}} c^{(\iota)}_d \int_{\mathbb{R}^d} |\xi|^{2m-k} f_m(\xi)[\pi(\mathbf{W}^{\mathscr{A},\iota}_1) \otimes \cdots \otimes \pi(\mathbf{W}^{\mathscr{A},\iota}_m)]\, d\xi. \end{aligned} \tag{10.7}$$

Turning our attention to the right-hand side of (10.6), we express $W_j^{\mathscr{A}}(\xi)$ in terms of $W_j^{\mathscr{A},\iota} := \pi(\mathbf{W}_j^{\mathscr{A},\iota})$ (see (4.3) and (3.5)), and find

$$f_m[W_1^{\mathscr{A}}(\xi) \otimes \cdots \otimes W_m^{\mathscr{A}}(\xi)] = \sum_{\iota:\mathscr{A}\to\{1,\ldots,d\}} \prod_{j\in\mathscr{A}} \xi_{\iota(j)} f_m[W_1^{\mathscr{A},\iota} \otimes \cdots \otimes W_m^{\mathscr{A},\iota}].$$

Hence, by using (7.1),

$$\begin{aligned}(-1)^m &\int\limits_{\mathbb{R}^d} f_m(\xi)[W_1^{\mathscr{A}}(\xi) \otimes \cdots \otimes W_m^{\mathscr{A}}(\xi)]\,d\xi \\ &= (-1)^m \sum_{\iota:\mathscr{A}\to\{1,\ldots,d\}} c_d^{(\iota)} \int\limits_{\mathbb{R}^d} |\xi|^{2m-k} f_m(\xi)[W_1^{\mathscr{A},\iota} \otimes \cdots \otimes W_m^{\mathscr{A},\iota}]\,d\xi \end{aligned} \tag{10.8}$$

The theorem follows by combining (10.7) with (10.8). □

Appendix A. Comments on the accompanying python program

Accompanying this paper is a python script that computes $I_k = I_k(\lambda_l(x)\Delta + \sum_i \lambda_l(a_i)D_i + \lambda_l(a))$ for any $k \in \mathbb{Z}_+$ in terms of multiple operator integrals with arguments in $C^\infty(\mathbb{T}_\theta^d)$. The program can also be found on the Github page https://github.com/TDHvanNuland/I_k.

The program outputs an identity (formatted in latex) with I_k on the left-hand side and an expression on the right-hand side with explicit dependency on d. The program can be easily adjusted to match the output type one prefers.

The last line of the program fixes the value of k. For example, to compute I_2 one can replace the last line

```
print_I(4)
```

with the line

```
print_I(2)
```

and run the program, for example by opening a terminal, navigating to the correct directory, and typing

```
python3 I_k.py
```

(any installed version of python should work). The output should be as follows.

$$-\pi^{-d/2} I_2 = \sum_i \left(2T^x_{F^{[3]}_{2,d}}(x, D_i x, D_i x) + T^x_{F^{[2]}_{2,d}}(x, D_i D_i x) + T^x_{F^{[2]}_{2,d}}(a_i, D_i x) + T^x_{F^{[1]}_{2,d}}(a/d) \right)$$

$$+\sum_i \frac{1}{d}\Bigg(4T^x_{F^{[4]}_{2,d}}(x,D_ix,x,D_ix)+4T^x_{F^{[3]}_{2,d}}(x,D_ix,D_ix)+8T^x_{F^{[4]}_{2,d}}(x,x,D_ix,D_ix)$$
$$+4T^x_{F^{[3]}_{2,d}}(x,x,D_iD_ix)+2T^x_{F^{[3]}_{2,d}}(x,D_ix,a_i)+2T^x_{F^{[2]}_{2,d}}(x,D_ia_i)$$
$$+2T^x_{F^{[3]}_{2,d}}(x,a_i,D_ix)+2T^x_{F^{[3]}_{2,d}}(a_i,x,D_ix)+T^x_{F^{[2]}_{2,d}}(a_i,a_i)\Bigg)$$

Computing I_4 in this way produces the 1046 terms in an instant, and computing I_6 takes about 10 minutes on an Intel(R) Core(T) i9-10900 CPU @ 2.80GHz, and produces 140845 terms (of course excluding sums over the indices $i, j, k, \ldots$, as otherwise the amount of terms depends on d).

Appendix B. Supplementary material

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.jfa.2024.110754.

Data availability

The python code file "`I_k.py`" has been shared at the "Attach file" step.

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