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Heat trace for Laplace type operators with non-scalar symbols

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Abstract

For an elliptic selfadjoint operator $P = -[u^{\mu\nu}\partial_\mu\partial_\nu + v^\nu\partial_\nu + w]$ acting on a fiber bundle over a compact Riemannian manifold, where $u^{\mu\nu}, v^\mu, w$ are $N \times N$-matrices, we develop a method to compute the heat-trace coefficients a_r which allows to get them by a pure computational machinery. It is exemplified in any even dimension by the value of a_1 written both in terms of $u^{\mu\nu} = g^{\mu\nu}u, v^\mu, w$ or diffeomorphic and gauge invariants. We also address the question: when is it possible to get explicit formulae for a_r?

Keywords: Heat kernel, non minimal operator, asymptotic heat trace, Laplace type operator
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2000 MSC: 58J35, 35J47, 81T13, 46L87

1. Introduction

We consider a compact Riemannian manifold (M, g) without boundary and of dimension d together with the nonminimal differential operator

$$P := -[u^{\mu\nu}(x)\partial_\mu\partial_\nu + v^\nu(x)\partial_\nu + w(x)]. \tag{1.1}$$

which is a differential operator on a smooth vector bundle V over M of fiber $\mathbb{C}^N$ where $u^{\mu\nu}$, v^ν, w are $N \times N$-matrices valued functions. This bundle is endowed with a hermitean metric. We work in a local trivialization of V over an open subset of M which is also a chart on M with coordinates (x^μ). In this trivialization, the adjoint for the hermitean metric corresponds to the adjoint of matrices and the trace on endomorphisms on V becomes the usual trace tr on matrices. Since we want P to be a selfadjoint and elliptic operator on $L^2(M, V)$, we first assume that $u^{\mu\nu}(x)\,\xi_\mu\xi_\nu$ is a positive definite matrix in M_N:

$$u^{\mu\nu}(x)\,\xi_\mu\xi_\nu \text{ has only strictly positive eigenvalues for any } \xi \neq 0. \tag{1.2}$$

We may assume without loss of generality that $u^{\mu\nu} = u^{\nu\mu}$. In particular $u^{\mu\mu}$ is a positive matrix for each μ and each $u^{\mu\nu}$ is selfadjoint.

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The asymptotics of the heat-trace

$$\operatorname{Tr} e^{-tP} \underset{t\downarrow 0^+}{\sim} \sum_{r=0}^{\infty} a_r(P)\, t^{r-d/2} \tag{1.3}$$

exists by standard techniques (see [1, Section 1.8.1]), so we want to compute these coefficients $a_r(P)$.
While the spectrum of P is a priori inaccessible, the computation of few coefficients of this asymptotics is eventually possible. The related physical context is quite large: the operators P appeared in gauge field theories, string theory or the so-called non-commutative gravity theory (see for instance the references quoted in [2, 3, 4]). The knowledge of the coefficients a_r are important in physics. For instance, the one-loop renormalization in dimension four requires a_1 and a_2.

When the principal symbol of P is scalar ($u^{\mu\nu} = g^{\mu\nu}\mathbb{1}_N$), there are essentially two main roads towards the calculation of heat coefficients (with numerous variants): the first is analytical and based on elliptic pseudodifferential operators while the second is more concerned by the geometry of the Riemannian manifold M itself with the search for invariants or conformal covariance. Compared with the flourishing literature existing when the principal symbol is scalar, there are only few works when it is not. One can quote for instance the case of operators acting on differential forms [5, 6, 7, 8]. The first general results are in [9] or in the context of spin geometry using the Dirac operators or Stein-Weiss operators [10] also motivated by physics [2]. See also the approach in [11, 12, 13, 14, 15, 16, 17, 18, 19].
The present work has a natural algebraic flavor inherited from the framework of operators on Hilbert space comprising its own standard analytical part, so is related with the first road. In particular, it gives all ingredients to produce mechanically the heat coefficients. It is also inspired by the geometry *à la* Connes where $P = \mathcal{D}^2$ for a commutative spectral triple $(\mathcal{A}, \mathcal{H}, \mathcal{D})$, thus has a deep motivation for noncommutative geometry.

Let us now enter into few technical difficulties.
While the formula for $a_0(P)$ is easily obtained, the computation of $a_1(P)$ is much more involved. To locate some difficulties, we first recall the parametrix approach, namely the use of momentum space coordinates $(x, \xi) \in T^*_x M$:

$$\begin{aligned} d_2(x,\xi) &= u^{\mu\nu}(x)\, \xi_\mu \xi_\nu\,, \\ d_1(x,\xi) &= -i v^\mu(x)\, \xi_\mu\,, \\ d_0(x) &= -w(x). \end{aligned}$$

Then we can try to use the generic formula (see [5])

$$a_r(P) = \tfrac{1}{(2\pi)^d} \tfrac{1}{-i2\pi} \int dx\, d\lambda\, d\xi\, e^{-\lambda} \operatorname{tr}\left[b_{2r}(x,\xi,\lambda)\right] \tag{1.4}$$

where λ belongs to a anticlockwise curve $\mathcal{C}$ around $\mathbb{R}^+$ and $(x,\, \xi) \in T^*(M)$. Here the functions b_{2r} are defined recursively by

$$\begin{aligned} b_0(x,\xi,\lambda) &:= (d_2(x,\xi) - \lambda)^{-1}, \\ b_r(x,\xi,\lambda) &:= -\sum_{\substack{r=j+|\alpha|+2-k \\ j<r}} \tfrac{(-i)^{|\alpha|}}{\alpha!} (\partial_\xi^\alpha b_j)(\partial_x^\alpha d_k)\, b_0. \end{aligned}$$

The functions b_{2r}, even for $r=1$, generate typically terms of the form

$$\mathrm{tr}[A_1(\lambda)B_1A_2(\lambda)B_2A_3(\lambda)\cdots]$$

where all matrices $A_i(\lambda)=(d_2(x,\xi)-\lambda)^{-n_i}$ commute but do not commute a priori with B_i, so that the integral in λ is quite difficult to evaluate in an efficient way. Of course, one can use the spectral decomposition $d_2=\sum_i \lambda_i\,\pi_i$ (depending on x and ξ) to get,

$$\sum_{i_1,i_2,i_3,\dots}\Big[\int_{\lambda\in\mathcal{C}} d\lambda\, e^{-\lambda}\,(\lambda_{i_1}-\lambda)^{-n_{i_1}}(\lambda_{i_2}-\lambda)^{-n_{i_2}}(\lambda_{i_3}-\lambda)^{-n_{i_3}}\cdots\Big]\,\mathrm{tr}(\pi_{i_1}B_1\pi_{i_2}B_2\pi_{i_3}\cdots). \quad (1.5)$$

While the λ-integral is easy via residue calculus, the difficulty is then to recombine the sum. This approach is conceptually based on an approximation of the resolvent $(P-\lambda)^{-1}$.

Because of previous difficulties, we are going to follow another strategy, using a purely functional approach for the kernel of e^{-tP} which is based on the Volterra series (see [20, p. 78],[4, Section 1.17.2]). This approach is not new and has been used for the same purpose in [9, 2, 3].

However our strategy is more algebraic and more in the spirit of rearrangement lemmas worked out in [21, 22]. In particular we do not go through the spectral decomposition of $u^{\mu\nu}$ crucially used in [9] (although in a slightly more general case than the one of Section 4). To explain this strategy, we need first to fix a few notation points.

Let $K(t,x,x')$ be the kernel of e^{-tP} where P is as in (1.1) and satisfies (1.2). Then

$$\begin{aligned}\mathrm{Tr}[e^{-tP}] &= \int dx\ \mathrm{tr}[K(t,x,x)],\\ K(t,x,x) &= \tfrac{1}{(2\pi)^d}\int d\xi\, e^{-ix.\xi}\,(e^{-tP}\,e^{ix.\xi}).\end{aligned}$$

When f is a matrix-valued function on M, we get

$$\begin{aligned}-P(e^{ix.\xi}f)(x) &= \Big(e^{ix.\xi}\,[-u^{\mu\nu}\xi_\mu\xi_\nu+2iu^{\mu\nu}\xi_\mu\partial_\nu+iv^\mu\xi_\mu+w(x)]f\Big)(x)\\ &= -\Big(e^{ix.\xi}\,[H+K+P]f\Big)(x)\end{aligned}$$

where we used

$$H(x,\xi) := u^{\mu\nu}(x)\,\xi_\mu\xi_\nu\,, \quad (1.6)$$
$$K(x,\xi) := -i\xi_\mu[v^\mu(x)+2u^{\mu\nu}(x)\,\partial_\nu]. \quad (1.7)$$

Thus H is the principal symbol of P and it is non-scalar for non-trivial matrices $u^{\mu\nu}$.

If $\mathbb{1}(x)=\mathbb{1}$ is the unit matrix valued function, we get $e^{-tP}e^{ix.\xi}=e^{ix.\xi}\,e^{-t(H+K+P)}\,\mathbb{1}$, so that, after the change of variables $\xi\to t^{1/2}\xi$, the heat kernel can be rewritten as

$$K(t,x,x)=\tfrac{1}{(2\pi)^d}\int d\xi\, e^{-t(H+K+P)}\,\mathbb{1}=\tfrac{1}{t^{d/2}}\tfrac{1}{(2\pi)^d}\int d\xi\, e^{-H-\sqrt{t}K-tP}\,\mathbb{1}. \quad (1.8)$$

A repetitive application of Duhamel formula (or Lagrange's variation of constant formula) gives the Volterra series (also known to physicists as Born series):

$$e^{A+B}=e^A+\sum_{k=1}^{\infty}\int_0^1 ds_1\int_0^{s_1}ds_2\cdots\int_0^{s_{k-1}}ds_k\ e^{(1-s_1)A}\,B\,e^{(s_1-s_2)A}\cdots e^{(s_{k-1}-s_k)A}\,B\,e^{s_kA}\,.$$

Since this series does not necessarily converge for unbounded operators, we use only its first terms to generate the asymptotics (1.3) from (1.8). When $A = -H$ and $B = -\sqrt{t}K - tP$, it yields for the integrand of (1.8)

$$\begin{aligned} e^{-H-\sqrt{t}K-tP}\mathbb{1} = \Big(& e^{-H} - \sqrt{t}\int_0^1 ds_1\, e^{(s_1-1)H}\, K\, e^{-s_1 H} \\ & + t\Big[\int_0^1 ds_1 \int_0^{s_1} ds_2\, e^{(s_1-1)H}\, K\, e^{(s_2-s_1)H}\, K\, e^{-s_2 H} - \int_0^1 ds_1\, e^{(s_1-1)H}\, P\, e^{-s_1 H}\Big] \\ & + \mathcal{O}(t^2)\Big)\mathbb{1}. \end{aligned} \tag{1.9}$$

After integration in ξ, the term in $\sqrt{t}$ is zero since K is linear in ξ while H is quadratic in ξ, so that

$$\operatorname{tr} K(t,x,x) \underset{t\downarrow 0}{\simeq} \tfrac{1}{t^{d/2}}[a_0(x) + t\, a_1(x) + \mathcal{O}(t^2)]$$

with the local coefficients

$$a_0(x) = \operatorname{tr} \tfrac{1}{(2\pi)^d} \int d\xi\, e^{-H(x,\xi)}, \tag{1.10}$$

$$\begin{aligned} a_1(x) = \operatorname{tr} \tfrac{1}{(2\pi)^d} \int d\xi \Big[\int_0^1 ds_1 \int_0^{s_1} ds_2\, e^{(s_1-1)H}\, K\, e^{(s_2-s_1)H}\, K\, e^{-s_2 H}\Big] \\ - \operatorname{tr} \tfrac{1}{(2\pi)^d} \int d\xi\, [\int_0^1 ds_1\, e^{(s_1-1)H}\, P\, e^{-s_1 H}] \end{aligned} \tag{1.11}$$

where the function $\mathbb{1}$ has been absorbed in the last $e^{-s_i H}$.
The coefficients $a_0(P)$ and $a_1(P)$ are obtained after an integration in x. Since we will not perform that integration which converges when manifold M is compact, we restrict to $a_r(x)$.

We now briefly explain how we can compute $a_r(P)$. Expanding K and P in $a_r(x)$, one shows in Section 2 that all difficulties reduce to compute algebraic expressions like (modulo the trace)

$$\tfrac{1}{(2\pi)^d} \int d\xi \int_0^1 ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{k-1}} ds_k\; e^{(s_1-1)H}\, B_1\, e^{(s_2-s_1)H}\, B_2 \cdots B_k\, e^{-s_k H} \tag{1.12}$$

where the B_i are $N \times N$-matrices equal to $u^{\mu\nu}$, v^μ, w or their derivatives of order two at most. Moreover, we see (1.12) as an M_N-valued operator acting on the variables $(B_1, \ldots, B_k)$ which precisely allows to focus on the integrations on ξ and s_i independently of these variables. Then we first compute the integration in ξ, followed by the iterated integrations in s_i. The main result of this section is (2.18) which represents the most general operator used in the computation of a_r. We end up Section 2 by a summary of the method. We show that the previously mentioned integrations are manageable in Section 3. Actually, we prove that we can reduce the computations to few universal integrals and count the exact number of them which are necessary to get $a_r(x)$ in arbitrary dimension. In Section 4, we reduce to the case $u^{\mu\nu} = g^{\mu\nu}u$ where u is a positive matrix and explicitly compute the local coefficient a_1 in Theorem 4.3 in terms of $(u,\, v^\mu,\, w)$. Looking after geometric invariants like for instance the scalar curvature of M, we swap the variables $(u,\, v^\mu,\, w)$ with some others based on a given connection A on V. This allows to study the diffeomorphic invariance and covariance under the gauge group of the bundle V. The coefficient a_1 can then be simply written in any

even dimension in terms of a covariant derivative (combining A and Christoffel symbols). In Section 5, we use our general results to address the following question: is it possible to get explicit formulae for a_r avoiding the spectral decomposition like (1.5)? We show that the answer is negative when d is odd. Finally, the case $u^{\mu\nu} = g^{\mu\nu}u + X^{\mu\nu}$ is considered as an extension of $u^{\mu\nu} = g^{\mu\nu}\mathbb{1} + X^{\mu\nu}$ which appeared in the literature.

2. Formal computation of $a_r(P)$

This section is devoted to show that the computation of $a_r(x)$ as (1.11) reduces to the one of the terms as in (1.12). Since a point $x \in M$ is fixed here, we forget to mention it, but many of the structures below are implicitly defined as functions of x.

For $k \in \mathbb{N}$, let Δ_k be the k-simplex

$$\Delta_k := \{s = (s_0, \cdots s_k) \in \mathbb{R}_+^{k+1} \,|\, 0 \le s_k \le s_{k-1} \le \cdots \le s_2 \le s_1 \le s_0 = 1\},$$
$$\Delta_0 := \varnothing \text{ by convention.}$$

We use the algebra M_N of $N \times N$-complex matrices.
Denote by $M_N[\xi, \partial]$ the complex vector space of polynomials both in $\xi = (\xi_\mu) \in \mathbb{R}^d$ and $\partial = (\partial_\mu)$ which are M_N-valued differential operators and polynomial in ξ; for instance, P, K, $H \in M_N[\xi, \partial]$ with P of order zero in ξ and two in ∂, K of order one in ξ and ∂, and H of order two in ξ and zero in ∂.

For any $k \in \mathbb{N}$, define a map $f_k(\xi) : M_N[\xi, \partial]^{\otimes^k} \to M_N[\xi, \partial]$, evidently related to (1.12), by

$$f_k(\xi)[B_1 \otimes \cdots \otimes B_k] := \int_{\Delta_k} ds\, e^{(s_1-1)H(\xi)}\, B_1\, e^{(s_2-s_1)H(\xi)}\, B_2 \cdots B_k\, e^{-s_k H(\xi)}, \tag{2.1}$$

$$f_0(\xi)[a] := a\, e^{-H(\xi)}, \quad \text{for } a \in \mathbb{C} =: M_N^{\otimes^0}. \tag{2.2}$$

Here, by convention, each ∂_μ in $B_i \in M_N[\xi, \partial]$ acts on all its right remaining terms. Remark that the map $\xi \mapsto f_k(\xi)$ is even.
We first rewrite (1.9) in these notations (omitting the ξ-dependence):

$$\begin{aligned} e^{-H-\sqrt{t}K-tP}\mathbb{1} &= e^{-H} + \sum_{k=1}^{\infty}(-1)^k f_k[(\sqrt{t}K + tP) \otimes \cdots \otimes (\sqrt{t}K + tP)] \\ &= e^{-H} \\ &\quad - t^{1/2} f_1[K] \\ &\quad + t(f_2[K \otimes K] - f_1[P]) \\ &\quad + t^{3/2}(f_2[K \otimes P] + f_2[P \otimes K] - f_3[K \otimes K \otimes K]) \\ &\quad + t^2(f_2[P \otimes P] - f_3[K \otimes K \otimes P] - f_3[K \otimes P \otimes K] - f_3[P \otimes K \otimes K]) \\ &\quad + \mathcal{O}(t^2). \end{aligned} \tag{2.3}$$

Since all powers of t in $(2n+1)/2$ have odd powers of $\xi_{\mu_1} \cdots \xi_{\mu_p}$ (with odd p), the ξ-integrals in (1.12) will be zero since f_k is even in ξ, so only

$$a_0(x) = \operatorname{tr} \tfrac{1}{(2\pi)^d} \int d\xi\, f_0[1], \tag{2.4}$$

$$a_1(x) = \operatorname{tr} \tfrac{1}{(2\pi)^d} \int d\xi\, (f_2[K \otimes K] - f_1[P]), \tag{2.5}$$

$$a_2(x) = \operatorname{tr} \tfrac{1}{(2\pi)^d} \int d\xi\, (f_2[P \otimes P] - f_3[K \otimes K \otimes P] - f_3[K \otimes P \otimes K] - f_3[P \otimes K \otimes K])$$

etc survive.
Our first (important) step is to erase the differential operator aspect of K and P as variables of f_k to obtain variables in the space $M_N[\xi]$ of M_N-valued polynomials in ξ: because a ∂ contained in B_i will apply on $e^{(s_{i+1}-s_i)H}B_{i+1}\cdots B_k e^{-s_kH}$, by a direct use of Leibniz rule and the fact that

$$\partial\, e^{-sH} = -\int_0^s ds_1\, e^{(s_1-s)H}\,(\partial H)\, e^{-s_1H}, \tag{2.6}$$

we obtain the following

Lemma 2.1 *When all B_j are in $M_N[\xi,\partial]$, the functions f_k for $k\in\mathbb{N}^*$ satisfy*

$$\begin{aligned} f_k(\xi)[B_1\otimes\cdots\otimes B_i\partial\otimes\cdots\otimes B_k] &= \sum_{j=i+1}^{k} f_k(\xi)[B_1\otimes\cdots\otimes(\partial B_j)\otimes\cdots\otimes B_k] \\ &\quad - \sum_{j=i}^{k} f_{k+1}(\xi)[B_1\otimes\cdots\otimes B_j\otimes(\partial H)\otimes B_{j+1}\otimes\cdots\otimes B_k]. \end{aligned} \tag{2.7}$$

Proof By definition (omitting the ξ-dependence)

$$\begin{aligned} &f_k[B_1\otimes\cdots\otimes B_i\partial\otimes\cdots\otimes B_k] \\ &\qquad = \int_{\Delta_k} ds\, e^{(s_1-1)H}B_1\, e^{(s_2-s_1)H}\, B_2\cdots B_i\partial(e^{(s_{i+1}-s_i)H}B_{i+1}\cdots B_k\, e^{-s_kH}). \end{aligned}$$

The derivation ∂ acts on each factor in the parenthesis:
– On the argument B_j, $j\geq i+1$, which gives the first term of (2.7).
– On a factor $e^{(s_{j+1}-s_j)H}$ for $i\leq j\leq k-1$, we use (2.6)

$$\partial\, e^{(s_{j+1}-s_j)H} = -\int_0^{s_j-s_{j+1}} ds'\, e^{s'+s_{j+1}-s_j)H}\,(\partial H)\, e^{-s'H} = -\int_{s_{j+1}}^{s_j} ds\, e^{(s-s_j)H}\,(\partial H)\, e^{(s_{j+1}-s)H}$$

with $s=s'+s_{j+1}$, so that in the integral, one obtains the term

$$\begin{aligned} -\int_0^1 ds_1\int_0^{s_1} ds_2\cdots\int_0^{s_{k-1}}\int_{s_{j+1}}^{s_j} ds\, e^{(s_1-1)H}B_1e^{(s_2-s_1)H}B_2\cdots \\ \cdots B_je^{(s-s_j)H}(\partial H)\, e^{(s_{j+1}-s)H}B_{j+1}\cdots B_k\, e^{-s_kH}). \end{aligned}$$

Since, as directly checked, $\int_0^1 ds_1\cdots\int_0^{s_{k-1}} ds_k\int_{s_j+1}^{s_j} ds = \int_{\Delta_{k+1}} ds'$ with $s'_j=s_j$ for $j\leq i-1$, $s'_i=s$ and $s'_j=s_{j-1}$ for $j\geq i+1$, this term is $-f_{k+1}[B_1\otimes\cdots\otimes B_j\otimes(\partial H)\otimes B_{j+1}\otimes\cdots\otimes B_k]$.
– Finally, on the factor e^{-s_kH}, one has $\partial\, e^{-s_kH} = -\int_0^{s_k} e^{(s-s_k)H}\,(\partial H)\, e^{-sH}$ which gives the last term: $-f_{k+1}[B_1\otimes\cdots\otimes B_k\otimes(\partial H)]$. ■

Thus (2.3) reduces to compute $f_k[B_1\otimes\cdots\otimes B_k]$ where $B_i\in M_N[\xi]$.
Our second step is now to take care of the ξ-dependence: by hypothesis, each B_i in the tensor product $B_1\otimes\cdots\otimes B_k$ has the form $\sum B^{\mu_1\cdots\mu_{\ell_i}}\,\xi_{\mu_1}\cdots\xi_{\mu_{\ell_i}}$ with $B^{\mu_1\cdots\mu_{\ell_i}}\in M_N$, so that $B_1\otimes\cdots\otimes B_k$ is a sum of terms like $\mathbb{B}_k^{\mu_1\cdots\mu_\ell}\,\xi_{\mu_1}\cdots\xi_{\mu_\ell}$ where $\mathbb{B}_k^{\mu_1\cdots\mu_\ell}\in M_N^{\otimes^k}$. As a consequence, by linearity of f_k in each variable, computation of a_r requires only to evaluate terms like

$$\tfrac{1}{(2\pi)^d}\int d\xi\,\xi_{\mu_1}\cdots\xi_{\mu_\ell}\, f_k(\xi)[\,\mathbb{B}_k^{\mu_1\cdots\mu_\ell}]\in M_N \quad \text{with } \mathbb{B}_k^{\mu_1\cdots\mu_\ell}\in M_N^{\otimes^k}, \tag{2.8}$$

and we may assume that $\ell = 2p$, $p \in \mathbb{N}$.

The next step in our strategy is now to rewrite the f_k appearing in (2.8) in a way which is independent of the variables $\mathbb{B}_k^{\mu_1 \cdots \mu_\ell}$, a rewriting obtained in (2.11). Then the driving idea is to show firstly that such f_k can be computed and secondly that its repeated action on all variables which pop up by linearity (repeat that K has two terms while P has three terms augmented by the action of derivatives, see for instance (1.11)) is therefore a direct computational machinery.

For such rewriting we need a few definitions justified on the way.

For $k \in \mathbb{N}$, define the (finite-dimensional) Hilbert spaces

$$\mathcal{H}_k := M_N^{\otimes^k}, \quad \mathcal{H}_0 := \mathbb{C},$$

endowed with the scalar product

$$\langle A_1 \otimes \cdots \otimes A_k, B_1 \otimes \cdots \otimes B_k \rangle_{\mathcal{H}_k} := \mathrm{tr}(A_1^* B_1) \cdots \mathrm{tr}(A_k^* B_k), \quad \langle a_0, b_0 \rangle_{\mathcal{H}_0} := \overline{a}_0 b_0,$$

so each M_N is seen with its Hilbert–Schmidt norm and $\|A_1 \otimes \cdots \otimes A_k\|^2_{\mathcal{H}_k} = \prod_{j=1}^k \mathrm{tr}(A_j^* A_j)$.

We look at (2.8) as the action of the operator $\frac{1}{(2\pi)^d} \int d\xi \, \xi_{\mu_1} \cdots \xi_{\mu_l} \, f_k(\xi)$ acting on the finite dimensional Hilbert space $\mathcal{H}_k$.

Denote by $\mathcal{B}(E, F)$ the set of bounded linear operators between the vector spaces E and F and let $\mathcal{B}(E) := \mathcal{B}(E, E)$. For $k \in \mathbb{N}$, let

$$\begin{aligned}
&\widehat{\mathcal{H}}_k := \mathcal{H}_{k+1}, \text{ so } \widehat{\mathcal{H}}_0 = M_N\,, && \\
&\mathbf{m} : \widehat{\mathcal{H}}_k \to M_N\,, && \mathbf{m}(B_0 \otimes \cdots \otimes B_k) := B_0 \cdots B_k \ \text{ (multiplication of matrices)}, \\
&\kappa : \mathcal{H}_k \to \widehat{\mathcal{H}}_k\,, && \kappa(B_1 \otimes \cdots \otimes B_k) := \mathbb{1} \otimes B_1 \otimes \cdots \otimes B_k\,, \\
&\iota : M_N^{\otimes^{k+1}} \to \mathcal{B}(\mathcal{H}_k, M_N), && \iota(A_0 \otimes \cdots \otimes A_k)[B_1 \otimes \cdots \otimes B_k] := A_0 B_1 A_1 \cdots B_k A_k\,, \\
&\iota : M_N \to \mathcal{B}(\mathbb{C}, M_N), && \iota(A_0)[a] := a A_0\,, \\
&\rho : M_N^{\otimes^{k+1}} \to \mathcal{B}(\widehat{\mathcal{H}}_k), && \rho(A_0 \otimes \cdots \otimes A_k)[B_0 \otimes \cdots \otimes B_k] := B_0 A_0 \otimes \cdots \otimes B_k A_k.
\end{aligned}$$

For $A \in M_N$ and $k \in \mathbb{N}$, define the operators

$$\begin{aligned}
&R_i(A) : \widehat{\mathcal{H}}_k \to \widehat{\mathcal{H}}_k \ \text{ for } i = 0, \ldots, k \\
&R_i(A)[B_0 \otimes \cdots \otimes B_k] := B_0 \otimes \cdots \otimes B_i A \otimes \cdots \otimes B_k.
\end{aligned}$$

Thus

$$\rho(A_0 \otimes \cdots \otimes A_k) = R_0(A_0) \cdots R_k(A_k). \tag{2.9}$$

As shown in Proposition A.1, ι is an isomorphism. The links between the three spaces $M_N^{\otimes^{k+1}}$, $\mathcal{B}(\widehat{\mathcal{H}}_k)$ and $\mathcal{B}(\mathcal{H}_k, M_N)$ are summarized in the following commutative diagram where $(\mathbf{m} \circ \kappa^*)(C)[B_1 \otimes \cdots \otimes B_k] = \mathbf{m}(C[\mathbb{1} \otimes B_1 \otimes \cdots \otimes B_k])$:

$$\begin{tikzcd}
 & \mathcal{B}(\widehat{\mathcal{H}}_k) \arrow[d, "m \circ \kappa^*"] \\
M_N^{\otimes k+1} \arrow[ur, "\rho"] \arrow[r, "\simeq", "\iota"'] & \mathcal{B}(\mathcal{H}_k, M_N)
\end{tikzcd} \tag{2.10}$$

For any matrix $A \in M_N$ and $s \in \Delta_k$, define

$$\begin{aligned} c_k(s,A) &:= (1-s_1)\, A \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} \,+\, (s_1 - s_2)\, \mathbb{1} \otimes A \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} \\ &\qquad + \cdots + \,(s_{k-1} - s_k)\, \mathbb{1} \otimes \cdots \otimes A \otimes \mathbb{1} \,+\, s_k\, \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes A, \\ c_0(s,A) &:= A \end{aligned}$$

where the tensor products have $k+1$ terms, so that $c_k(s,A) \in M_N^{\otimes k+1}$.
This allows a compact notation since now

$$f_k(\xi) = \int_{\Delta_k} ds\ \iota[e^{-\xi_\alpha \xi_\beta\, c_k(s,u^{\alpha\beta})}] \in \mathcal{B}(\mathcal{H}_k, M_N), \qquad \text{with } f_0(\xi) = \iota(e^{-\xi_\alpha \xi_\beta u^{\alpha\beta}}), \tag{2.11}$$

and these integrals converge because the integrand is continuous and the domain Δ_k is compact.
Since we want to use operator algebra techniques, with the help of $c_k(s,A) \in M_N^{\otimes k+1}$, it is useful to lift the computation of (2.11) to the (finite dimensional C^*-algebra) $\mathcal{B}(\widehat{\mathcal{H}}_k)$ as viewed in diagram (2.10). Thus, we define

$$C_k(s,A) := \rho(c_k(s,A)) \in \mathcal{B}(\widehat{\mathcal{H}}_k),$$

and then, by (2.9)

$$C_k(s,A) = (1-s_1)\, R_0(A) + (s_1 - s_2)\, R_1(A) + \cdots + (s_{k-1} - s_k)\, R_{k-1}(A) + s_k\, R_k(A).$$

Remark 2.2 All these distinctions between $\mathcal{H}_k$ and $\widehat{\mathcal{H}}_k$ or $c_k(s,A)$ and $C_k(s,A)$ seem innocent so tedious. But we will see later on that the distinctions between the different spaces in (2.10) play a conceptual role in the difficulty to compute the coefficients a_r. Essentially, the computations and results take place in $\mathcal{B}(\widehat{\mathcal{H}}_k)$ and not necessarily in the subspace $M_N^{\otimes k+1} \subset \mathcal{B}(\widehat{\mathcal{H}}_k)$ (see (2.18) for instance). □

Given a diagonalizable matrix $A = C\,\mathrm{diag}(\lambda_1, \ldots, \lambda_n)\, C^{-1} \in M_N$, let $C^{ij} := C E^{ij} C^{-1}$ for $i,j = 1, \ldots, n$ where the E^{ij} form the elementary basis of M_N defined by $[E^{ij}]_{kl} := \delta_{ik}\, \delta_{jl}$.
We have the easily proved result:

Lemma 2.3 *We have*
i) $R_i(A_1 A_2) = R_i(A_2) R_i(A_1)$ *and* $[R_i(A_1),\, R_j(A_2)] = 0$ *when* $i \neq j$.
ii) $R_i(A)^* = R_i(A^*)$.
iii) When A *is diagonalizable,* $AC^{ij} = \lambda_i\, C^{ij}$ *and* $C^{ij} A = \lambda_j\, C^{ij}$.
Thus, all operators $R_i(A)$ *on* $\widehat{\mathcal{H}}_k$ *for any* $k \in \mathbb{N}$ *have common eigenvectors*

$$R_i(A)[C^{i_0 j_0} \otimes \cdots \otimes C^{i_k j_k}] = \lambda_{j_i}\, C^{i_0 j_0} \otimes \cdots \otimes C^{i_k j_k},$$

and same spectra as A.
In particular, there are strictly positive operators if A *is a strictly positive matrix.*

This means that $C_k(s,A) \geq 0$ if $A \geq 0$ and $s \in \Delta_k$, and this justifies the previous lift. Now, evaluating (2.11) amounts to compute the following operators in $\mathcal{B}(\widehat{\mathcal{H}}_k)$:

$$T_{k,p}(x) := \tfrac{1}{(2\pi)^d} \int_{\Delta_k} ds \int d\xi\, \xi_{\mu_1} \cdots \xi_{\mu_{2p}}\, e^{-\xi_\alpha \xi_\beta\, C_k(s,u^{\alpha\beta}(x))} : \widehat{\mathcal{H}}_k \to \widehat{\mathcal{H}}_k, \quad p \in \mathbb{N},\ k \in \mathbb{N}. \tag{2.12}$$

$$T_{0,0}(x) := \tfrac{1}{(2\pi)^d} \int d\xi\ e^{-\xi_\alpha \xi_\beta u^{\alpha\beta}(x)} \in M_N \simeq \rho(M_N) \subset \mathcal{B}(\widehat{\mathcal{H}}_0), \tag{2.13}$$

where $T_{k,p}$ depends on x through $u^{\alpha\beta}$ only. Their interest stems from the fact they are independent of arguments $B_0 \otimes \cdots \otimes B_k \in \widehat{\mathcal{H}}_k$ on which they are applied, so are the corner stones of this work. Using (2.10), the precise link between $T_{k,p}$ and $f_k(\xi)$ is

$$\mathbf{m} \circ \kappa^* \circ T_{k,p} = \tfrac{1}{(2\pi)^d} \int d\xi\, \xi_{\mu_1} \cdots \xi_{\mu_{2p}}\, f_k(\xi). \tag{2.14}$$

The fact that $T_{k,p}$ is a bounded operator is justified by the following

Lemma 2.4 *The above integrals* (2.12) *and* (2.13) *converge and* $T_{k,p} \in \mathcal{B}(\widehat{\mathcal{H}}_k)$.

Proof We may assume $k \in \mathbb{N}^*$ since for $k = 0$, same arguments apply.
For any strictly positive matrix A with minimal eigenvalues $\lambda_{\min}(A) > 0$, Lemma 2.3 shows that, for any $s \in \Delta_k$,

$$C_k(s, A) \geq [(1 - s_1)\lambda_{\min}(A) + (s_1 - s_2)\lambda_{\min}(A) + \cdots + s_k\lambda_{\min}(A)]\, \mathbb{1}_{\widehat{\mathcal{H}}_k} = \lambda_{\min}(A)\, \mathbb{1}_{\widehat{\mathcal{H}}_k}.$$

We claim that the map $\xi \in \mathbb{R}^d \mapsto \lambda_{min}(\xi_\alpha \xi_\beta u^{\alpha\beta})$ is continuous: the maps $\xi \in \mathbb{R}^d \mapsto \xi_\alpha \xi_\beta u^{\alpha\beta}$ and $0 < a \in \mathcal{B}(\widehat{\mathcal{H}}_k) \mapsto \inf(\text{spectrum}(a)) = \|a^{-1}\|$ are continuous (the set of invertible matrices is a Lie group).
We use spherical coordinates $\xi \in \mathbb{R}^d \to (|\xi|, \sigma) \in \mathbb{R}_+ \times S^{d-1}$, where $\sigma := |\xi|^{-1}\xi$ is in the Euclidean sphere S^{d-1} endowed with its volume form $d\Omega$.
Then $\lambda_{min}(\xi_\alpha \xi_\beta u^{\alpha\beta}) = |\xi|^2 \lambda_{min}(\sigma_\alpha \sigma_\beta u^{\alpha\beta}) > 0$ (remark that $\sigma_\alpha \sigma_\beta u^{\alpha\beta}$ is a strictly positive matrix). Thus $c := \inf\{\lambda_{min}(\sigma_\alpha \sigma_\beta u^{\alpha\beta}) \,|\, \sigma \in S^{d-1}\} > 0$ by compactness of the sphere. The usual operator-norm of $\widehat{\mathcal{H}}_k$ applied on the above integral $T_{k,p}$, satisfies

$$\begin{aligned}
\|T_{k,p}\| &\leq \int_{\Delta_k} ds \int_{\sigma \in S^{d-1}} d\Omega_g(\sigma) \int_0^\infty dr\, \|r^{d-1} r^{2p}\, \sigma_{\mu_1} \cdots \sigma_{\mu_{2p}}\, e^{-r^2 c\, \mathbb{1}_{\widehat{\mathcal{H}}_k}}\| \\
&\leq \int_{\Delta_k} ds \int_{\sigma \in S^{d-1}} d\Omega_g(\sigma) \int_0^\infty dr\, r^{d-1+2p}\, e^{-r^2 c} = \text{vol}(\Delta_k)\, \text{vol}(S_g^{d-1})\, \tfrac{\Gamma(d/2+p)}{2}\, c^{-d/2-p}. \qquad \blacksquare
\end{aligned}$$

For the ξ-integration of (2.12), we use again spherical coordinates, but now $\xi = r\,\sigma$ with $r = (g^{\mu\nu}\xi_\mu \xi_\nu)^{1/2}$, $\sigma = r^{-1}\xi \in S_g^{d-1}$ (this sphere depends on $x \in M$ through $g(x)$) and define

$$u[\sigma] := u^{\mu\nu}\sigma_\mu \sigma_\nu$$

which is a positive definite matrix for any $\sigma \in S_g^{d-1}$. Thus we get

$$\begin{aligned}
T_{k,p} &= \tfrac{1}{(2\pi)^d} \int_{\Delta_k} ds \int_{S_g^{d-1}} d\Omega_g(\sigma)\, \sigma_{\mu_1} \cdots \sigma_{\mu_{2p}} \int_0^\infty dr\, r^{d-1+2p}\, e^{-r^2 C_k(s, u[\sigma])} \\
&= \tfrac{\Gamma(d/2+p)}{2(2\pi)^d} \int_{S_g^{d-1}} d\Omega_g(\sigma)\, \sigma_{\mu_1} \cdots \sigma_{\mu_{2p}} \int_{\Delta_k} ds\; C_k(s, u[\sigma])^{-(d/2+p)}.
\end{aligned} \tag{2.15}$$

Thus, we have to compute the s-integration $\int_{\Delta_k} ds\, C_k(s, u[\sigma])^{-\alpha}$ for $\alpha \in \frac{1}{2}\mathbb{N}^*$. We do that via functional calculus, using Lemma 2.3 iii), by considering the following integrals

$$\begin{aligned}
I_{\alpha,k}(r_0, r_1, \ldots, r_k) &:= \int_{\Delta_k} ds\, [(1 - s_1)r_0 + (s_1 - s_2)r_1 + \cdots + s_k r_k]^{-\alpha} \\
&= \int_{\Delta_k} ds\, [r_0 + s_1(r_1 - r_0) + \cdots + s_k(r_k - r_{k-1})]^{-\alpha}
\end{aligned} \tag{2.16}$$

$$I_{\alpha,0}(r_0) := r_0^{-\alpha}, \text{ for } \alpha \neq 0, \tag{2.17}$$

where $0 \neq r_i \in \mathbb{R}_+$ corresponds, in the functional calculus, to positive operator $R_i(u[\sigma])$. Such integrals converge for any $\alpha \in \mathbb{R}$ and any $k \in \mathbb{N}^*$, even if it is applied above only to $\alpha = d/2 + k - r \in \frac{1}{2}\mathbb{N}$. Nevertheless for technical reasons explained below, it is best to define $I_{\alpha,k}$ for an arbitrary $\alpha \in \mathbb{R}$.
In short, the operator $T_{k,p}$ is nothing else than the operator in $\mathcal{B}(\widehat{\mathcal{H}}_k)$

$$T_{k,p} = \tfrac{\Gamma(d/2+p)}{2(2\pi)^d} \int_{S_g^{d-1}} d\Omega_g(\sigma)\, \sigma_{\mu_1} \cdots \sigma_{\mu_{2p}}\, I_{d/2+p,k}\Big(R_0(u[\sigma]), R_1(u[\sigma]), \ldots, R_k(u[\sigma])\Big). \tag{2.18}$$

Remark that $T_{k,p}$ depends on x via $u[\sigma]$ and the metric g.

Remark 2.5 We pause for a while to make a connection with the previous work [9]. There, the main hypothesis on the matrix $u^{\mu\nu}\xi_\mu\xi_\nu$ is that all its eigenvalues are positive multiples of $g^{\mu\nu}\xi_\mu\xi_\nu$ for any $\xi \neq 0$. Under this hypothesis, we can decompose spectrally $u[\sigma] = \sum_i \lambda_i \pi_i[\sigma]$ where the eigenprojections π_i depends on σ but the associated eigenvalues λ_i do not. Then, operator functional calculus gives

$$I_{d/2+p,k}\Big(R_0(u[\sigma]), \ldots, R_k(u[\sigma])\Big) = \sum_{i_0,\ldots,i_k} I_{d/2+p,k}(\lambda_{i_0}, \ldots, \lambda_{i_k})\, R_0(\pi_{i_0}[\sigma]) \cdots R_k(\pi_{i_k}[\sigma]) \tag{2.19}$$

and

$$T_{k,p} = \tfrac{\Gamma(d/2+p)}{2(2\pi)^d} \sum_{i_1,\ldots,i_k} I_{d/2+p,k}(\lambda_{i_0}, \ldots, \lambda_{i_k}) \int_{S_g^{d-1}} d\Omega_g(\sigma)\, \sigma_{\mu_1} \cdots \sigma_{\mu_{2p}}\, R_0(\pi_{i_0}[\sigma]) \cdots R_k(\pi_{i_k}[\sigma])$$

where all $\pi_{i_0}[\sigma], \ldots, \pi_{i_k}[\sigma]$ commute as operators in $\mathcal{B}(\widehat{\mathcal{H}}_k)$. However, we do not try to pursue in that direction since it is not very explicit due to the difficult last integral on the sphere; also we remind that we already gave up in the introduction the use of the eigenprojections for the same reason. Instead, we give for instance a complete computation of a_1 in Section 4 directly in terms of matrices $u^{\mu\nu}, v^\mu, w$, avoiding this spectral splitting in the particular case where $u^{\mu\nu} = g^{\mu\nu}u$ for a positive matrix u. □

In conclusion, as claimed in the introduction, the above approach really reduces the computation of all $a_r(x)$ for an arbitrary integer r to the control of operators $T_{k,p}$ which encode all difficulties since, once known, their actions on an arbitrary variable $B_1 \otimes \cdots \otimes B_k$ with $B_i \in M_n$ are purely mechanical. For instance in any dimension of M, the calculus of $a_1(x)$ needs only to know, $T_{1,0}$, $T_{2,1}$, $T_{3,2}$, $T_{4,3}$. More generally, we have the following

Lemma 2.6 *For any dimension d of the manifold M and $x \in M$, given $r \in \mathbb{N}$, the computation of $a_r(P)$ needs exactly to know each of the $3r+1$ operators $T_{k,k-r}$ where $r \leq k \leq 4r$ or equivalently to know $I_{d/2,r}$, $I_{d/2+1,r+1}, \ldots,$ $I_{d/2+3r,4r}$.*

Proof As seen in (2.3), using the linearity of f_k in each argument, we may assume that in $f_k[B_1 \otimes \cdots \otimes B_k]$ each argument B_i is equal to K or P, so generates $t^{1/2}$ or t in the asymptotic expansion. Let n_K and n_P the number of K and P for such f_k involved in $a_r(P)$. Since $a_r(P)$ is the coefficient of t^r, we have $\frac{1}{2}n_K + n_P = r$ and $k \geq r$. In particular, n_K much be even.

When $B_i = K = -i\xi_\mu[v^\mu(x) + 2u^{\mu\nu}(x)\,\partial_\nu]$, again by linearity, we may assume that the argument in $f(k,p) := f_k(\xi)[B_1(\xi) \otimes \cdots \otimes B_k(\xi)]$ is a polynomial of order $2p$ since odd order are cancelled out after the ξ-integration. In such $f(k,p)$, the number of ξ (in the argument) is equal to n_K, so that $p = \frac{1}{2}n_K$, and the number of derivations ∂ is $n_K + 2n_P$.

We count now all $f(k,p)$ involved in the computation of $a_r(P)$. We initiate the process with $(k,p) = (n_K + n_P, \frac{1}{2}n_K)$, so $k-p=r$ and after the successive propagation of ∂ as in Lemma 2.1, we end up with (k',p') where $k'-p'=r$: in (2.7), $k \to k+1$ while $p \to p+1$ since ∂H appears as a new argument. So $(k',p') = (k', k'-r)$ and the maximum of k' is $2n_K + 3n_P$. Here, $n_P = 0,\dots,r$ and $n_K = 0,\dots,2r$, so that the maximum is for $k' = 4r$.
All $f(k,k-r)$ with $r \le k \le 4r$ will be necessary to compute $a_r(P)$: Let k be such that $r \le k \le 3r$. Then a term $f(k,k-r)$ will be obtained by the use of Lemma 2.1 applied on $f_r[u^{\mu_1\nu_1}\partial_{\mu_1}\partial_{\nu_1} \otimes \cdots \otimes u^{\mu_r\nu_r}\partial_{\mu_r}\partial_{\nu_r}]$ with an action of $k-r$ derivatives on the e^{sH} and the reminder on the B_i. The same argument, applied to $f_{2r}[\xi_{\mu_1}u^{\mu_1\nu_1}\partial_{\nu_1} \otimes \cdots \otimes \xi_{\mu_{2r}}u^{\mu_{2r}\nu_{2r}}\partial_{\nu_{2r}}]$, also generates a term $f(k,k-r)$ when $2r \le k \le 4r$.
Finally, remark that we can swap the ξ-dependence of $f(k,p)$ into definition (2.12) of $T_{k,p}$ to end up with integrals which are advantageously independent of arguments B_i.

The case $r=0$ is peculiar: since $k=0$ automatically, we have only to compute $T_{0,0}$ in (2.13) which gives $a_0(x)$ by (1.10).
The link between the T's and the I is given in (2.18).
The preceding reasoning is independent of the dimension d. ■

Of course, in an explicit computation of $a_r(x)$, each of these $3r+1$ operators $T_{k,k-r}$ can be used several times since applied on different arguments $B_1 \otimes \cdots \otimes B_k$. The integral $I_{d/2+p,k}$ giving T_k, p in (2.18) will be explicitly computed in Section 3.

We now list the terms of $a_1(x)$. Using the shortcuts

$$\bar{v} := \xi_\mu v^\mu, \qquad \bar{u}^\nu := \xi_\mu u^{\mu\nu},$$

starting from (2.5) and applying Lemma 2.1, we get

$$-f_1[P] = -f_2[u^{\mu\nu} \otimes \partial_\mu\partial_\nu H] + 2f_3[u^{\mu\nu} \otimes \partial_\mu H \otimes \partial_\nu H] - f_2[v^\mu \otimes \partial_\mu H] + f_1[w], \tag{2.20}$$

$$\begin{aligned} f_2[K \otimes K] = &-f_2[\bar{v} \otimes \bar{v}] + 2f_3[\bar{v} \otimes \bar{u}^\nu \otimes \partial_\nu H] - 2f_2[\bar{u}^\mu \otimes \partial_\mu \bar{v}] + 2f_3[\bar{u}^\mu \otimes \partial_\mu H \otimes \bar{v}] \\ &+ 2f_3[\bar{u}^\mu \otimes \bar{v} \otimes \partial_\mu H] + 4f_3[\bar{u}^\mu \otimes \partial_\mu \bar{u}^\nu \otimes \partial_\nu H] + 4f_3[\bar{u}^\mu \otimes \bar{u}^\nu \otimes \partial_\mu\partial_\nu H] \\ &- 4f_4[\bar{u}^\mu \otimes \partial_\mu H \otimes \bar{u}^\nu \otimes \partial_\nu H] - 4f_4[\bar{u}^\mu \otimes \bar{u}^\nu \otimes \partial_\mu H \otimes \partial_\nu H] \\ &- 4f_4[\bar{u}^\mu \otimes \bar{u}^\nu \otimes \partial_\nu H \otimes \partial_\nu H]. \end{aligned} \tag{2.21}$$

This represents 14 terms to compute for getting $a_1(x)$.

Summary of the method: We pause here to summarize the chosen method. To compute $a_r(x)$, we first expand K and P in (2.3) in terms of matrix valued differential operators which are arguments of M_N-valued operators $f_k(\xi)$, and then we remove all derivative operators from the arguments using the generalized Leibniz rule (2.7). This generates a sum of terms like (2.8). Then, the method splits along two independent computational axes: the first one is to collect all the arguments $\mathbb{B}_k^{\mu_1\cdots\mu_\ell}$ produced by (2.7); the second one is to compute the operators obtained by integration of $f_k(\xi)$ with respect to ξ, which, thanks to (2.10) and (2.14), requires to compute some operators $T_{k,p}$. The latter operators are written in (2.18) using spherical coordinates for that ξ-integral, in terms of universal integrals $I_{d/2+p,k}$ defining operators depending only on $u^{\mu\nu}$ and the metric g. In the generic situation, the links between $T_{k,p}$, $I_{d/2+p,k}$, and f_k are given in (2.18) and (2.14), but another link between f_k and $I_{d/2+p,k}$ will be given in (4.4) in a particular case where the integrals (2.18) can be fully computed. The last step of the method is to collect the (matrix) traces of evaluations of operators (second axe) on the arguments (first axe): $a_r(x)$ is just a sum of such contributions. Moreover, Lemma 2.6 determines the number of integrals $I_{d/2+p,k}$ to compute to get $a_r(x)$.

3. Integral computations of $I_{\alpha,k}$

We begin with few interesting remarks on $I_{\alpha,k}$ defined in (2.16) and (2.17):

Proposition 3.1 *Properties of functions $I_{\alpha,k}$:*
i) Recursive formula valid for $1 \neq \alpha \in \mathbb{R}$ and $k \in \mathbb{N}^*$:

$$I_{\alpha,k}(r_0,\dots,r_k) = \tfrac{1}{(\alpha-1)}(r_{k-1}-r_k)^{-1}[I_{\alpha-1,k-1}(r_0,\dots,r_{k-2},r_k) - I_{\alpha-1,k-1}(r_0,\dots,r_{k-1})]. \quad (3.1)$$

(The abandoned case $I_{1,k}$ is computed in Proposition 3.3.)
ii) Symmetry with respect to last two variables:

$$I_{\alpha,k}(r_0,\dots,r_{k-1},r_k) = I_{\alpha,k}(r_0,\dots,r_k,r_{k-1}).$$

iii) Continuities:
The functions $I_{\alpha,k} : (\mathbb{R}_+^*)^{k+1} \to \mathbb{R}_+^*$ are continuous for all $\alpha \in \mathbb{R}$.
For any $(r_0,\dots,r_{k-1},r_k) \in (\mathbb{R}_+^*)^{k+1}$, the map $\alpha \in \mathbb{R}^+ \mapsto I_{\alpha,k}(r_0,\dots,r_{k-1},r_k)$ is continuous.
iv) Special values: for any $\alpha \in \mathbb{R}$ and $k \in \mathbb{N}$,

$$I_{\alpha,k}(\underbrace{r_0,\cdots,r_0}_{k+1}) = \tfrac{1}{k!}\, r_0^{-\alpha}. \quad (3.2)$$

Proof i) In $I_{\alpha,k}(r_0,\dots,r_k) = \int_0^1 ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{k-1}} ds_k\, [r_0+s_1(r_1-r_0)+\cdots+s_k(r_k-r_{k-1})]^{-\alpha}$, the last integral is equal to

$$\tfrac{1}{(\alpha-1)}(r_{k-1}-r_k)^{-1}\,[(r_0+s_1(r_1-r_0)+\cdots+s_{k-1}(r_{k-1}-r_{k-2})+s_{k-1}(r_k-r_{k-1}))^{-(\alpha-1)} \\ -(r_0+s_1(r_1-r_0)+\cdots+s_{k-1}(r_{k-1}-r_{k-2}))^{-(\alpha-1)}]$$

which gives the claimed relation. One checks directly from the definition (2.16) of $I_{\alpha+1,1}(r_0,r_1)$ that (3.1) is satisfied for the given $I_{\alpha,0}$.

ii) $I_{\alpha,1}(r_0,r_1) = \int_0^1 ds\, r_0 + s(r_1-r_0)]^{-\alpha} = \int_0^1 ds'\,[r_1+s'(r_0-r_1)]^{-\alpha} = I_{\alpha,1}(r_1,r_0)$ after the change of variable $s \to s' = 1-s$. The symmetry follows now using (3.1) by a recurrence process.

iii) The map $g(s,\bar r) := [(1-s_1)r_0+(s_1-s_2)r_1+\cdots+s_kr_k]^{-\alpha} > 0$ is continuous at the point $\bar r \in (\mathbb{R}_+^*)^{k+1}$ and uniformly bounded in a small ball $\mathcal{B}$ around $\bar r$ since then we have $g(s,\bar r) \le \max(r_{min}^{-|\alpha|}, r_{max}^{|\alpha|})$ where $r_{min \text{ or } max} := \min$ or $\max\{r_i \,|\, \bar r \in \mathcal{B}\} > 0$. Thus, since the integration domain Δ_k is compact, by Lebesgue's dominated convergence theorem, we get the continuity of $I_{\alpha,k}$.
It remains to prove the continuity of $\alpha \mapsto I_{\alpha,k}(r_0,\dots,r_{k-1},r_k)$: If $r_{min} := \min r_i > 0$, then $(1-s_1)r_0+(s_1-s_2)r_1+\cdots+s_kr_k \ge r_{min}$, so that $((1-s_1)r_0+(s_1-s_2)r_1+\cdots+s_kr_k)^{-\alpha} \le r_{min}^{-\alpha}$ and choosing $a = \min(1/2, r_{min}), r_{min}^{-\alpha} \le a^{-\alpha} \le a^{-\beta_1}$ for $\alpha \in (\beta_0,\beta_1)$, we can apply again Lebesgue's dominated convergence theorem.

(iv) Using the very definition (2.16),

$$I_{\alpha,k}(r_0,\dots,r_0) = \int_{\Delta_k} ds\, r_0^{-\alpha} = \mathrm{vol}(\Delta_k) r_0^{-\alpha} = \tfrac{1}{k!} r_0^{-\alpha}. \qquad \blacksquare$$

From Lemma 2.6 and (2.18), the computation of $a_r(P)$, for $r \geq 1$ (since a_0 is known already by (4.5)) in spatial dimension $d \geq 1$, requires all $I_{d/2+k-r,k}$ for $r \leq k \leq 4r$. The sequence $I_{d/2,r}, I_{d/2+1,r+1}, \ldots, I_{d/2+3r,4r}$ belongs to the same recursive relation (3.1), except if there is a $s \in \mathbb{N}$ such that $d/2 + s = 1$, which can only happen with $d = 2$ and $s = 0$ (see Case 1 below). The computation of this sequence requires then to compute $I_{d/2,r}$ as the root of (3.1).

The function $I_{d/2,r}$ can itself be computed using (3.1) when this relation is relevant.
Case 1: d is even and $d/2 \leq r$, recursive sequence (3.1) fails at $I_{1,r-d/2+1}$:

$$I_{1,r-d/2+1} \to I_{2,r-d/2+2} \to \cdots \to \underbrace{I_{d/2,r} \to I_{d/2+1,r+1} \to \cdots \to I_{d/2+3r,4r}}_{\text{used to compute } a_r(x)} . \tag{3.3}$$

Case 2: d is even and $r < d/2$, relation (3.1) never fails and

$$I_{d/2-r,0} \to I_{d/2-r+1,1} \to I_{d/2-r+2,2} \to \cdots \to \underbrace{I_{d/2,r} \to I_{d/2+1,r+1} \to \cdots \to I_{d/2+3r,4r}}_{\text{used to compute } a_r(x)} . \tag{3.4}$$

Case 3: d is odd, relation (3.1) never fails and

$$I_{d/2-r,0} \to I_{d/2-r+1,1} \to I_{d/2-r+2,2} \to \cdots \to \underbrace{I_{d/2,r} \to I_{d/2+1,r+1} \to \cdots \to I_{d/2+3r,4r}}_{\text{used to compute } a_r(x)} . \tag{3.5}$$

In the latter case, the root is $I_{\alpha,0}$ with $\alpha = d/2 - r$ half-integer, positive or negative and both situation have to be considered separately.

The recursive relation (3.1), which for $I_{\alpha,k}$ follows from the integration on the k-simplex Δ_k, has a generic solution:

Proposition 3.2 *Given $\alpha_0 \in \mathbb{R}$, $k_0 \in \mathbb{N}$ and a function $F : \mathbb{R}_+^* \to \mathbb{R}_+^*$, let the function $J_{\alpha_0+k_0,k_0} : (\mathbb{R}_+^*)^{k+1} \to \mathbb{R}_+^*$ be defined by*

$$J_{\alpha_0+k_0,k_0}(r_0, \ldots, r_k) := c_{\alpha_0+k_0,k_0} \sum_{i=0}^{k_0} \Big[\prod_{\substack{j=0 \\ j\neq i}}^{k_0} (r_i - r_j)^{-1} \Big] F(r_i).$$

i) Ascending chain: Then, all functions $J_{\alpha_0+k,k}$ obtained by applying the recurrence formula (3.1) for any $k \in \mathbb{N}$, $k \geq k_0$ have the same form:

$$J_{\alpha_0+k,k}(r_0, \ldots, r_k) := c_{\alpha_0+k,k} \sum_{i=0}^{k} \Big[\prod_{\substack{j=0 \\ j\neq i}}^{k} (r_i - r_j)^{-1} \Big] F(r_i) \tag{3.6}$$

with

$$c_{\alpha_0+k,k} = \tfrac{(-1)^{k-k_0}}{(\alpha_0+k_0)\cdots(\alpha_0+k-1)}\, c_{\alpha_0+k_0,k_0} \quad \text{for } k > k_0 . \tag{3.7}$$

ii) Descending chain: when $\alpha_0 \in \mathbb{R}\backslash\{-\mathbb{N}\}$, the functions $J_{\alpha_0+k,k}$ defined by (3.6) for $k \in \mathbb{N}^*$ starting with $k_0 = 0$, the root $F(r_0) = J_{\alpha_0,0}(r_0)$ and

$$c_{\alpha_0+k,k} = \tfrac{(-1)^k}{\alpha_0(\alpha_0+1)\cdots(\alpha_0+k-1)} \tag{3.8}$$

satisfy (3.1).

Proof i) It is sufficient to show that

$$X := \tfrac{1}{\alpha-1}(r_{\ell-1}-r_\ell)^{-1}[J_{\alpha-1,\ell-1}(r_0,\dots,r_{\ell-2},r_\ell) - J_{\alpha-1,\ell-1}(r_0,\dots,r_{\ell-1})].$$

has precisely the form (3.6) for $\ell = k_0+1$ and $\alpha = \alpha_0+k_0+1$. We have

$$X = \tfrac{c_{\alpha-1,\ell-1}}{\alpha-1}(r_{\ell-1}-r_\ell)^{-1}\Big[\sum_{i=0}^{\ell-2}\Big(\prod_{\substack{j=0\\ j\neq i}}^{\ell-2}(r_i-r_j)^{-1}\Big)(r_i-r_\ell)^{-1}F(r_i) + \prod_{j=0}^{\ell-2}(r_\ell-r_i)^{-1}F(r_\ell)$$
$$-\sum_{i=0}^{\ell-2}\Big(\prod_{\substack{j=0\\ j\neq i}}^{\ell-2}(r_i-r_j)^{-1}\Big)(r_i-r_{\ell-1})^{-1}F(r_i) - \prod_{j=0}^{\ell-2}(r_{\ell-1}-r_i)^{-1}F(r_{\ell-1})\Big]. \quad (3.9)$$

We can combine the two sums on $i=0,\dots,\ell-2$ as:

$$\sum_{j=0}^{\ell-2}\Big(\prod_{\substack{j=0\\ j\neq i}}^{\ell-2}(r_i-r_j)^{-1}\Big)[(r_i-r_\ell)^{-1}-(r_i-r_{\ell-1})^{-1}]\,F(r_i) = (r_\ell-r_{\ell-1})\sum_{j=0}^{\ell-2}\Big(\prod_{\substack{j=0\\ j\neq i}}^{\ell}(r_i-r_j)^{-1}\Big)F(r_i).$$

Including $(r_{\ell-1}-r_\ell)^{-1}$, the others terms in (3.9) correspond to $[\prod_{\substack{j=0\\ j\neq i}}^{\ell}(r_i-r_j)^{-1}]\,F(r_i)$ for $i=\ell-1$ and $i=\ell$ (up to a sign), so that

$$X = -\tfrac{c_{\alpha-1,\ell-1}}{\alpha-1}\sum_{j=0}^{\ell}\Big(\prod_{\substack{j=0\\ j\neq i}}^{\ell}(r_i-r_j)^{-1}\Big)F(r_i)$$

which yields $c_{\alpha_0+k_0+1,k_0+1} = -\frac{1}{\alpha_0+k_0}c_{\alpha_0+k_0,k_0}$ and so the claim (3.7).

ii) It is the same argument with $k_0=0$ and the hypothesis $\alpha_0\notin -\mathbb{N}$ guarantees the existence of (3.8) and moreover $c_{\alpha_0,0}=1$. ■

Proposition 3.2 exhibits the general solution of Cases 2 and 3 in (3.4) and (3.5) (with $\alpha_0 = d/2-r$, for d even and $\alpha_0>0$, or for d odd), with, for both, $F(r_0) = I_{d/2-r,0}(r_0) = r_0^{-\alpha_0}$, so that

$$I_{d/2-r+k,k}(r_0,\dots,r_k) = \tfrac{(-1)^k}{(d/2-r)(d/2-r+1)\cdots(d/2-r+k-1)}\sum_{i=0}^{k}\Big[\prod_{\substack{j=0\\ j\neq i}}^{k}(r_i-r_j)^{-1}\Big]r_i^{-(d/2-r)}. \quad (3.10)$$

To control the reminder Case 1 of chain (3.3) where $\alpha_0\in-\mathbb{N}$ (so for d even and $\alpha_0 = d/2-r\le 0$), we need to compute the functions $I_{k-\alpha_0,k}$ for $\alpha_0\in\{0,1,\cdots,k-1\}$. This is done below and shows surprisingly enough that the generic solution of Proposition 3.2 holds true also for a different function $F(r_0)$. Actually, this is simple consequence of the fact that, despite its presentation in (3.10), the RHS has no poles as function of r.

Corollary 3.3 *Case 1: d even and $d/2\le r$ (so $\alpha_0 = d/2-r\le 0$).*
For any $k\in\mathbb{N}^*$, and $\ell = r-d/2\in\{0,1,\cdots,k-1\}$

$$I_{k-\ell,k}(r_0,\dots,r_k) = \tfrac{(-1)^{k-\ell-1}}{(k-\ell-1)!\,\ell!}\sum_{i=0}^{k}\Big[\prod_{\substack{j=0\\ j\neq i}}^{k}(r_i-r_j)^{-1}\Big]r_i^{\ell}\log r_i. \quad (3.11)$$

Proof Let $d/2 = m \in \mathbb{N}^*$. Then using the continuity of Proposition 3.1 with (3.10)

$$\begin{aligned}
I_{k-\ell,k}(r_0,\dots,r_k) &= \lim_{r\to m+\ell} I_{m-r+k,k}(r_0,\dots,r_{n+k}) \\
&= \lim_{r\to m+\ell} \tfrac{(-1)^k}{(m-r)\cdots(m-r+k-1)} \sum_{i=0}^{k} \Big[\prod_{\substack{j=0\\ j\neq i}}^{k} (r_i-r_j)^{-1}\Big] r_i^{-(m-r)} \\
&= \big[\lim_{r\to m+\ell} \tfrac{(-1)^{k-1}}{(m-r)\cdots(m-r+\ell-1)} \tfrac{1}{(m-r+\ell+1)\cdots(m-r+k-1)}\big] \\
&\qquad\qquad \lim_{r\to m+\ell} \sum_{i=0}^{k} \Big[\prod_{\substack{j=0\\ j\neq i}}^{k} (r_i-r_j)^{-1}\Big] r_i^{\ell} \tfrac{1}{r-(m+\ell)} r_i^{r-(m+\ell)} \\
&= \tfrac{(-1)^{k-\ell-1}}{(k-\ell-1)!\,\ell!} \sum_{i=0}^{k} \Big[\prod_{\substack{j=0\\ j\neq i}}^{k} (r_i-r_j)^{-1}\Big] r_i^{\ell} \log r_i
\end{aligned}$$

where we used (A.1) for the second limit in last equality. ■

The next propositions compute explicitly Case 3 and then Case 2, and the result is not written as in (3.10) where denominators in $r_i - r_j$ appear. This allows to deduce algorithmically (*i.e.* without any integration) the sequence $I_{d/2,r}, I_{d/2+1,r+1}, \dots, I_{d/2+3r,4r}$.

Proposition 3.4 *Case 3: d is odd.*
If $d/2 - r = \ell + 1/2$ with $\ell \in \mathbb{N}$, the root and its follower are

$$\begin{aligned}
&I_{\ell+1/2,0}(r_0) = r_0^{-\ell-1/2}, \\
&I_{\ell+3/2,1}(r_0,r_1) = \tfrac{2}{2\ell+1}(\sqrt{r_0}\sqrt{r_1}\,)^{-2\ell-1}(\sqrt{r_0}+\sqrt{r_1}\,)^{-1} \sum_{0\le l_1\le 2\ell} \sqrt{r_0}^{\,l_1}\,\sqrt{r_1}^{\,2\ell-l_1},
\end{aligned}$$

while if $d/2 - r = -\ell - 1/2$ with $\ell \in \mathbb{N}$, the root and its follower are

$$\begin{aligned}
&I_{-\ell-1/2,0}(r_0) = r_0^{\ell+1/2}, \\
&I_{-\ell+1/2,1}(r_0,r_1) = \tfrac{2}{2\ell+1}(\sqrt{r_0}+\sqrt{r_1}\,)^{-1} \sum_{0\le l_1\le 2\ell} \sqrt{r_0}^{\,l_1}\,\sqrt{r_1}^{\,2\ell-l_1}.
\end{aligned}$$

Proof Using (3.1) and (2.17), we get when $\ell \ge 0$

$$\begin{aligned}
I_{\ell+3/2,1}(r_0,r_1) &= \tfrac{1}{\ell+1/2}(r_0-r_1)^{-1}[I_{\ell+1/2,0}(r_1) - I_{\ell+1/2,0}(r_0)] \\
&= \tfrac{2}{2\ell+1}(\sqrt{r_0}-\sqrt{r_1}\,)^{-1}(\sqrt{r_0}+\sqrt{r_1}\,)^{-1}[r_1^{-\ell-1/2} - r_0^{-\ell-1/2}]
\end{aligned}$$

where the term in bracket is

$$\begin{aligned}
r_1^{-\ell-1/2} - r_0^{-\ell-1/2} &= (\sqrt{r_0}\sqrt{r_1}\,)^{-2\ell-1}[r_0^{2\ell+1} - r_1^{2\ell+1}] \\
&= (\sqrt{r_0}\sqrt{r_1}\,)^{-2\ell-1}(\sqrt{r_0}-\sqrt{r_1}\,) \sum_{0\le l_1\le 2\ell} \sqrt{r_0}^{\,l_1}\,\sqrt{r_1}^{\,2\ell-l_1},
\end{aligned}$$

which gives the result. Similar proof for the other equality. ■

This proposition exhibits only the two first terms of the recurrence chain in Case 3: similar formulae can be obtained at any level in which no $(r_i - r_j)^{-1}$ factors appear. Unfortunately, they are far more involved.

Proposition 3.5 *Case 2: d even and $r < d/2$.*
For $k \in \mathbb{N}^*$ and $\mathbb{N} \ni n = d/2 - r + k \geq k+1$,

$$\begin{aligned} &I_{n,k}(r_0,\dots,r_k) \\ &\quad= \tfrac{(r_0\cdots r_k)^{-1}}{(n-1)\cdots(n-k)} \sum_{\substack{0\leq l_k\leq l_{k-1}\leq\cdots \\ \cdots\leq l_1\leq n-(k+1)}} r_0^{l_1-(n-(k+1))}\, r_1^{l_2-l_1}\cdots r_{k-1}^{l_k-l_{k-1}}\, r_k^{-l_k} \qquad (3.12) \\ &\quad= \tfrac{(r_0\cdots r_k)^{-(n-k)}}{(n-1)\cdots(n-k)} \sum_{\substack{0\leq l_k\leq l_{k-1}\leq\cdots \\ \cdots\leq l_1\leq n-(k+1)}} r_0^{l_1}\, r_1^{l_2+(n-(k+1))-l_1}\cdots r_{k-1}^{l_k+(n-(k+1))-l_{k-1}}\, r_k^{(n-(k+1))-l_k}. \qquad (3.13) \end{aligned}$$

In (3.13), all exponents in the sum are positive while they are negative in (3.12). In particular

$$I_{n+k,k}(r_0,\dots,r_k) = \tfrac{(r_0\cdots r_k)^{-n}}{(n+k-1)\cdots(n+1)n} \sum_{\substack{0\leq l_k\leq l_{k-1}\leq\cdots \\ \cdots\leq l_1\leq n-1}} r_0^{l_1}\, r_1^{l_2+(n-1)-l_1}\cdots r_{k-1}^{l_k+(n-1)-l_{k-1}}\, r_k^{(n-1)-l_k}. \tag{3.14}$$

Proof The first and second equalities follow directly from the third that we prove now. Equality (3.14) is true for $k=1$ (the case $k=0$ is just the convention (2.17)) since

$$\begin{aligned} I_{n,1}(r_0,r_1) &= \int_0^1 ds_1\,(r_0+s_1(r_1-r_0))^{-n} = \tfrac{1}{n-1}(r_0-r_1)^{-1}[r_1^{-n+1}-r_0^{-n+1}] \\ &= \tfrac{1}{n-1}(r_0r_1)^{-n+1}\sum_{l_1=0}^{n-2} r_0^{l_1}r_1^{n-2-l_1}. \end{aligned}$$

Assuming (3.14) holds true for $l = 0,\dots,k-1$, formula (3.1) gives

$$\begin{aligned} &I_{n+k,k}(r_0,\dots,r_k) \\ &\quad= \tfrac{1}{n+k-1}(r_{k-1}-r_k)^{-1}\Big[I_{n+k-1,k-1}(r_0,\dots,r_{k-2},r_k) - I_{n+k-1,k-1}(r_0,\dots,r_{k-2},r_{k-1})\Big]. \end{aligned}$$

The term in bracket is

$$\begin{aligned} &\tfrac{(r_0\cdots r_{k-2}r_k)^{-n}}{(n+k-2)\cdots n} \sum_{\substack{0\leq l_{k-1}\leq l_{k-2}\leq\cdots \\ \cdots\leq l_1\leq n-1}} r_0^{l_1}r_1^{l_2+(n-1)-l_1}\cdots r_{k-2}^{l_{k-1}+(n-1)-l_{k-2}}r_k^{n-1-l_{k-1}} \\ -&\tfrac{(r_0\cdots r_{k-2}r_{k-1})^{-n}}{(n+k-2)\cdots n} \sum_{\substack{0\leq l_{k-1}\leq l_{k-2}\leq\cdots \\ \cdots\leq l_1\leq n-1}} r_0^{l_1}r_1^{l_2+(n-1)-l_1}\cdots r_{k-2}^{l_{k-1}+(n-1)-l_{k-2}}r_{k-1}^{n-1-l_{k-1}}. \end{aligned}$$

Thus

$$\begin{aligned} I_{n+k,k}(r_0,\dots,r_{k+1}) = \tfrac{(r_0\cdots r_{k-2})^{-n}}{(n+k-1)\cdots n} &\sum_{\substack{0\leq l_{k-1}\leq l_{k-2}\leq\cdots \\ \cdots\leq l_1\leq n-1}} r_0^{l_1}r_1^{l_2+(n-1)-l_1}\cdots r_{k-2}^{l_{k-1}+(n-1)-l_{k-2}} \\ &(r_{k-1}-r_k)^{-1}\Big[r_k^{-n}r_k^{n-1-l_{k-1}} - r_{k-1}^{-n}r_{k-1}^{(n-1)-l_{k-1}}\Big]. \end{aligned}$$

Since the last line is equal to

$$(r_{k-1}r_k)^{-1-l_{k-1}} \sum_{0\le l_k\le l_{k-1}} r_{k-1}^{l_k} r_k^{l_{k-1}-l_k} = (r_{k-1}r_k)^{-n} \sum_{0\le l_k\le l_{k-1}} r_{k-1}^{(n-1)+l_k-l_{k-1}} r_k^{(n-1)-l_k}$$

we have proved (3.14). ■

The interest of (3.14) is the fact that in (2.18) we have the following: for $B_0\otimes\cdots\otimes B_k\in\widehat{\mathcal{H}}_k$,

$$\begin{aligned} I_{n+k,k}\Big(R_0(u[\sigma]),\dots,R_k(u[\sigma])\Big)[B_0\otimes\cdots\otimes B_k] \\ = \tfrac{1}{(n+k-1)\cdots(n+1)n} \sum_{\substack{0\le l_k\le l_{k-1}\le\cdots \\ \cdots\le l_1\le n-1}} B_0\, u[\sigma]^{l_1-n}\otimes B_1\, u[\sigma]^{l_2-l_1-1}\otimes\cdots \\ \cdots\otimes B_{k-1}\, u[\sigma]^{l_k-l_{k-1}-1}\otimes B_k\, u[\sigma]^{-l_k-1}; \end{aligned} \tag{3.15}$$

or viewed as an operator in $\mathcal{B}(\mathcal{H}_k, M_N)$ (see diagram (2.10)):

$$\begin{aligned} &\mathbf{m}\circ\kappa^*\circ I_{n+k,k}\Big(R_0(u[\sigma]),\dots,R_k(u[\sigma])\Big)[B_1\otimes\cdots\otimes B_k] \\ &= \tfrac{1}{(n+k-1)\cdots(n+1)n} \sum_{\substack{0\le l_k\le l_{k-1}\le\cdots \\ \cdots\le l_1\le n-1}} u[\sigma]^{l_1-n} B_1\, u[\sigma]^{l_2-l_1-1} B_2\cdots B_{k-1}\, u[\sigma]^{l_k-l_{k-1}-1} B_k\, u[\sigma]^{-l_k-1}. \end{aligned}$$

While, if one wants to use directly (3.10) on $B_0\otimes\cdots\otimes B_k$, we face the difficulty to evaluate $[R_i(u)-R_j(u)]^{-1}[B_0\otimes\cdots\otimes B_k]$ in $\widehat{\mathcal{H}}_k$.

Another defect of (3.10) shared by (3.11) is that it suggests an improper behavior of integrals $I_{n+1,k+n}$ when two variables r_i are equal. But the continuity proved in Proposition 3.1 shows that this is just an artifact.

4. An example for $u^{\mu\nu} = g^{\mu\nu}u$

Here, we explicitly compute $a_1(x)$ assuming P satisfies (1.1) and (4.1).
Given a strictly positive matrix $u(x)\in M_N$ where $x\in(M,g)$, we satisfy Hypothesis 1.2 with

$$u^{\mu\nu}(x) := g^{\mu\nu}(x)\, u(x). \tag{4.1}$$

This implies that

$$H(x,\xi) = |\xi|^2_{g(x)}\, u(x) \text{ where } |\xi|^2_{g(x)} := g^{\mu\nu}(x)\,\xi_\mu\xi_\nu\,.$$

Of course the fact that $u[\sigma]=u$ is then independent of σ, simplifies considerably (2.18) since the integral in ξ can be performed. Thus we assume (4.1) from now on and (2.18) becomes

$$T_{k,p} = g_d\, G(g)_{\mu_1\dots\mu_{2p}}\, I_{d/2+p,k}\Big(R_0(u),R_1(u),\dots,R_k(u)\Big)\in\mathcal{B}(\widehat{\mathcal{H}}_k) \tag{4.2}$$

with (see [23, Section 1.1])

$$\begin{aligned} g_d &:= \tfrac{1}{(2\pi)^d}\int_{\mathbb{R}^d} d\xi\, e^{-|\xi|^2_{g(x)}} = \tfrac{\sqrt{|g|}}{2^d\,\pi^{d/2}}\,, \\ G(g)_{\mu_1\dots\mu_{2p}} &:= \tfrac{1}{(2\pi)^d\, g_d}\int d\xi\,\xi_{\mu_1}\cdots\xi_{\mu_{2p}}\, e^{-g^{\alpha\beta}\xi_\alpha\xi_\beta} \\ &= \tfrac{1}{2^{2p}\,p!}\Big(\sum_{\rho\in S_{2p}} g_{\mu_{\rho(1)}\mu_{\rho(2)}}\cdots g_{\mu_{\rho(2p-1)}\mu_{\rho(2p)}}\Big) = \tfrac{(2p)!}{2^{2p}\,p!}\, g_{(\mu_1\mu_2\dots\mu_{2p})} \end{aligned} \tag{4.3}$$

where $|g| := \det(g_{\mu\nu})$, S_{2p} is the symmetric group of permutations on $2p$ elements and the parenthesis in the index of g is the complete symmetrization over all indices.

Recall from Lemma 2.3 that if u has a spectral decomposition

$$u = \sum_{i=0}^{N-1} r_i E_i \,,$$

each $R_j(u)$ has the same spectrum as u.

Using the shortcuts

$$I_{d/2+p,k} := I_{d/2+p,k}\Big(R_0(u), \dots, R_k(u)\Big),$$

the formula (2.8) becomes simply

$$\begin{aligned}\tfrac{1}{(2\pi)^d}\int d\xi\, \xi_{\mu_1}\cdots\xi_{\mu_{2p}}\, f_k(\xi)[\,\mathbb{B}_k^{\mu_1\dots\mu_{2p}}] &= g_d\,(\mathbf{m}\circ\kappa^*\circ I_{d/2+p,k})[G(g)_{\mu_1\dots\mu_{2p}}\,\mathbb{B}_k^{\mu_1\dots\mu_{2p}}]\\ &= g_d\,(\mathbf{m}\circ I_{d/2+p,k})[\mathbb{1}\otimes G(g)_{\mu_1\dots\mu_{2p}}\,\mathbb{B}_k^{\mu_1\dots\mu_{2p}}]. \qquad (4.4)\end{aligned}$$

In particular, it is possible to compute the dimension-free contractions $G(g)_{\mu_1\dots\mu_{2p}}\,\mathbb{B}_k^{\mu_1\dots\mu_{2p}}$ before evaluating the result in the $I_{d/2+p,k}$'s.

For $a_0(x)$, we get

$$a_0(x) = \operatorname{tr}\tfrac{1}{(2\pi)^d}\int d\xi\, e^{-u(x)|\xi|^2_{g(x)}} = g_d(x)\ \operatorname{tr}[u(x)^{-d/2}]. \qquad (4.5)$$

In the sequel, we use frequently the following

Lemma 4.1 *For any $n_1, n_2, n_3 \in \mathbb{N}$, $A_1, A_2 \in M_N, \alpha \in \mathbb{R}^+$, and $k = n_1+n_2+n_3+2$, define*

$$X(A_1, A_2) := \operatorname{tr}(\mathbf{m}\circ I_{\alpha,k}[\mathbb{1}\otimes \underbrace{u\otimes\cdots\otimes u}_{n_1}\otimes A_1\,\underbrace{u\otimes\cdots\otimes u}_{n_2}\otimes A_2\otimes \underbrace{u\otimes\cdots\otimes u}_{n_3}]).$$

we have

$$X(A_1, A_2) = \sum_{r_0, r_1} r_0^{n_1+n_3}\, r_1^{n_2}\, I_{\alpha,k}(\underbrace{r_0,\cdots,r_0}_{n_1+1}, \underbrace{r_1,\cdots,r_1}_{n_2+1}, \underbrace{r_0,\cdots,r_0}_{n_3+1})\ \operatorname{tr}(E_0A_1E_1A_2) \qquad (4.6)$$

where E_i is the eigenprojection associated to eigenvalues r_i of u.
In particular,

$$\text{if } [A_1, u] = 0, \quad X(A_1, A_2) = \tfrac{1}{k!}\operatorname{tr}(u^{k-\alpha-2}A_1A_2). \qquad (4.7)$$

Proof The number $X(A_1, A_2)$ is equal to

$$\begin{aligned}&\sum_{r_i} I_{\alpha,k}(r_0,\dots,r_k)\operatorname{tr}\Big(\underbrace{E_0uE_1u\cdots E_{n_1}}_{n_1+1}A_1\underbrace{E_{n_1+1}uE_1u\cdots E_{n_1+n_2+1}}_{n_2+1}A_2\\ &\qquad\qquad\underbrace{E_{n_1+n_2+2}u\cdots uE_{n_1+n_2+n_3+2}}_{n_3+1}\Big)\\ &= \sum_{r_i} I_{\alpha,k}(r_0,\dots,r_k)\operatorname{tr}\Big(E_{n_1+n_2+2}u\cdots uE_{n_1+n_2+n_3+2}E_0uE_1u\cdots E_{n_1}A_1\\ &\qquad\qquad E_{n_1+1}uE_1u\cdots E_{n_1+n_2+1}A_2\Big)\\ &= \sum_{r_i} r_0^{n_1+n_3}r_1^{n_2}\, I_{\alpha,k}(\underbrace{r_0,\cdots,r_0}_{n_1+1}, \underbrace{r_1,\cdots,r_1}_{n_2+1}, \underbrace{r_0,\cdots,r_0}_{n_3+1})\operatorname{tr}(u^{n_1+n_3}E_0A_1u^{n_2}E_1A_2)\end{aligned}$$

yielding (4.6).
The particular case follows from $\mathrm{tr}(E_0A_1E_1A_2) = \delta_{0,1}\,\mathrm{tr}(E_0A_1A_2)$ and

$$I_{\alpha,k}(\underbrace{r_0,\cdots,r_0}_{k+1}) = \tfrac{1}{k!}\,r_0^{-\alpha}. \tag{4.8}$$

■

We also quote for further references the elementary

Corollary 4.2 *For any symmetric tensor $S^{ab} = S^{ba}$, any A_a, $A_b \in M_N$ and any function $g:\,(r_0,r_1)\in(\mathbb{R}_+^*)^2 \to \mathbb{R}$,*

$$\sum_{r_i} g(r_0,r_1)S^{ab}\,\mathrm{tr}(\pi_{r_0}A_a\pi_{r_1}A_b) = \sum_{r_i}\tfrac{1}{2}[g(r_0,r_1)+g(r_1,r_0)]\,S^{ab}\,\mathrm{tr}(\pi_{r_0}A_a\pi_{r_1}A_b). \tag{4.9}$$

We now divide the computation of $a_1(x)$ into several steps.

4.1. Collecting all the arguments

As a first step, we begin to collect all terms $\mathbb{B}_k^{\mu_1\cdots\mu_{2p}}$ of (4.4) due to the different variables appearing in (2.20) and (2.21), including their signs.

Variable in f_1: w.

Variables in f_2 without the common factor $\xi_{\mu_1}\xi_{\mu_2}$ and summation over μ_1,μ_2:

$$\begin{aligned}
-u^{\mu\nu}\otimes\partial_\mu\partial_\nu H \quad &\to \quad -g^{\mu\nu}(\partial_\mu\partial_\nu g^{\mu_1\mu_2})\,u\otimes u - 2g^{\mu\nu}(\partial_\mu g^{\mu_1\mu_2})\,u\otimes\partial_\nu u - g^{\mu\nu}g^{\mu_1\mu_2}\,u\otimes\partial_\mu\partial_\nu u\\
-v^\mu\otimes\partial_\mu H \quad &\to \quad -(\partial_\mu g^{\mu_1\mu_2})\,v^\mu\otimes u - g^{\mu_1\mu_2}\,v^\mu\otimes\partial_\mu u\\
-\bar v\otimes\bar v \quad &\to \quad -v^{\mu_1}\otimes v^{\mu_2}\\
-2\bar u^\mu\otimes\partial_\mu\bar v \quad &\to \quad -2g^{\mu\mu_1}\,u\otimes\partial_\mu v^{\mu_2}.
\end{aligned}$$

Variables in f_3 without the commun factor $\Pi_{i=1}^4\xi_{\mu_i}$ and summation over the μ_i:

$$\begin{aligned}
2u^{\mu\nu}\otimes\partial_\mu H\otimes\partial_\nu H \quad &\to \quad +2g^{\mu\nu}(\partial_\mu g^{\mu_1\mu_2})(\partial_\nu g^{\mu_3\mu_4})\,u\otimes u\otimes u\\
&\qquad +2g^{\mu\nu}(\partial_\mu g^{\mu_1\mu_2})g^{\mu_3\mu_4}\,u\otimes u\otimes\partial_\nu u\\
&\qquad +2g^{\mu\nu}g^{\mu_1\mu_2}(\partial_\nu g^{\mu_3\mu_4})\,u\otimes\partial_\mu u\otimes u\\
&\qquad +2g^{\mu\nu}g^{\mu_1\mu_2}g^{\mu_3\mu_4}\,u\otimes\partial_\mu u\otimes\partial_\nu u\\
2\bar v\otimes\bar u^\mu\otimes\partial_\mu H \quad &\to \quad +2g^{\mu\mu_2}(\partial_\mu g^{\mu_3\mu_4})\,v^{\mu_1}\otimes u\otimes u + 2g^{\mu\mu_2}g^{\mu_3\mu_4}\,v^{\mu_1}\otimes u\otimes\partial_\mu u\\
2\bar u^\mu\otimes\partial_\mu H\otimes\bar v \quad &\to \quad +2g^{\mu\mu_1}(\partial_\mu g^{\mu_2\mu_3})\,u\otimes u\otimes v^{\mu_4} + 2g^{\mu\mu_1}g^{\mu_2\mu_3}\,u\otimes\partial_\mu u\otimes v^{\mu_4}\\
2\bar u^\mu\otimes\bar v\otimes\partial_\mu H \quad &\to \quad +2g^{\mu\mu_1}(\partial_\mu g^{\mu_3\mu_4})\,u\otimes v^{\mu_2}\otimes u + 2g^{\mu\mu_1}g^{\mu_3\mu_4}\,u\otimes v^{\mu_2}\otimes\partial_\mu u\\
4\bar u^\mu\otimes\partial_\mu\bar u^\nu\otimes\partial_\nu H \quad &\to \quad +4g^{\mu\mu_1}(\partial_\mu g^{\nu\mu_2})(\partial_\nu g^{\mu_3\mu_4})\,u\otimes u\otimes u\\
&\qquad +4g^{\mu\mu_1}(\partial_\mu g^{\nu\mu_2})g^{\mu_3\mu_4}\,u\otimes u\otimes\partial_\nu u\\
&\qquad +4g^{\mu\mu_1}g^{\nu\mu_2}(\partial_\nu g^{\mu_3\mu_4})\,u\otimes\partial_\mu u\otimes u\\
&\qquad +4g^{\mu\mu_1}g^{\nu\mu_2}g^{\mu_3\mu_4}\,u\otimes\partial_\mu u\otimes\partial_\nu u\\
4\bar u^\mu\otimes\bar u^\nu\otimes\partial_\mu\partial_\nu H \quad &\to \quad +4g^{\mu\mu_1}g^{\nu\mu_2}(\partial_\mu\partial_\nu g^{\mu_3\mu_4})\,u\otimes u\otimes u\\
&\qquad +4g^{\mu\mu_1}g^{\nu\mu_2}(\partial_\mu g^{\mu_3\mu_4})\,u\otimes u\otimes\partial_\nu u\\
&\qquad +4g^{\mu\mu_1}g^{\nu\mu_2}(\partial_\nu g^{\mu_3\mu_4})\,u\otimes u\otimes\partial_\mu u\\
&\qquad +4g^{\mu\mu_1}g^{\nu\mu_2}g^{\mu_3\mu_4}\,u\otimes u\otimes\partial_\mu\partial_\nu u
\end{aligned}$$

Variables in f_4 without the commun factor $\Pi_{i=1}^{6}\xi_{\mu_i}$ and summation over the μ_i:

$$
\begin{aligned}
-4\bar{u}^\mu \otimes \partial_\mu H \otimes \bar{u}^\nu \otimes \partial_\nu H \quad &\to \quad -4g^{\mu\mu_1}(\partial_\mu g^{\mu_2\mu_3})g^{\nu\mu_4}(\partial_\nu g^{\mu_5\mu_6})\, u\otimes u\otimes u\otimes u \\
&\quad -4g^{\mu\mu_1}(\partial_\mu g^{\mu_2\mu_3})g^{\nu\mu_4}g^{\mu_5\mu_6}\, u\otimes u\otimes u\otimes \partial_\nu u \\
&\quad -4g^{\mu\mu_1}g^{\mu_2\mu_3}g^{\nu\mu_4}(\partial_\nu g^{\mu_5\mu_6})\, u\otimes \partial_\mu u\otimes u\otimes u \\
&\quad -4g^{\mu\mu_1}g^{\mu_2\mu_3}g^{\nu\mu_4}g^{\mu_5\mu_6}\, u\otimes \partial_\mu u\otimes u\otimes \partial_\nu u \\
-4\bar{u}^\mu \otimes \bar{u}^\nu \otimes \partial_\mu H \otimes \partial_\nu H \quad &\to \quad -4g^{\mu\mu_1}g^{\nu\mu_2}(\partial_\mu g^{\mu_3\mu_4})(\partial_\nu g^{\mu_5\mu_6})\, u\otimes u\otimes u\otimes u \\
&\quad -4g^{\mu\mu_1}g^{\nu\mu_2}(\partial_\mu g^{\mu_3\mu_4})g^{\mu_5\mu_6}\, u\otimes u\otimes u\otimes \partial_\nu u \\
&\quad -4g^{\mu\mu_1}g^{\nu\mu_2}g^{\mu_3\mu_4}(\partial_\nu g^{\mu_5\mu_6})\, u\otimes u\otimes \partial_\mu u\otimes u \\
&\quad -4g^{\mu\mu_1}g^{\nu\mu_2}g^{\mu_3\mu_4}g^{\mu_5\mu_6}\, u\otimes u\otimes \partial_\mu u\otimes \partial_\nu u \\
-4\bar{u}^\mu \otimes \bar{u}^\nu \otimes \partial_\nu H \otimes \partial_\mu H \quad &\to \quad -4g^{\mu\mu_1}g^{\nu\mu_2}(\partial_\nu g^{\mu_3\mu_4})(\partial_\mu g^{\mu_5\mu_6})\, u\otimes u\otimes u\otimes u \\
&\quad -4g^{\mu\mu_1}g^{\nu\mu_2}(\partial_\nu g^{\mu_3\mu_4})g^{\mu_5\mu_6}\, u\otimes u\otimes u\otimes \partial_\mu u \\
&\quad -4g^{\mu\mu_1}g^{\nu\mu_2}g^{\mu_3\mu_4}(\partial_\mu g^{\mu_5\mu_6})\, u\otimes u\otimes \partial_\nu u\otimes u \\
&\quad -4g^{\mu\mu_1}g^{\nu\mu_2}g^{\mu_3\mu_4}g^{\mu_5\mu_6}\, u\otimes u\otimes \partial_\nu u\otimes \partial_\mu u.
\end{aligned}
$$

A second and tedious step is now to do in (4.4) the metric contractions $G(g)_{\mu_1\dots\mu_{2p}}\,\mathbb{B}_k^{\mu_1\dots\mu_{2p}}$ for previous terms where the $G(g)_{\mu_1\dots\mu_{2p}}$ are given by:

$$G(g)_{\mu_1\mu_2} = \tfrac{1}{2}\, g_{\mu_1\mu_2}\,, \tag{4.10}$$

$$G(g)_{\mu_1\mu_2\mu_3\mu_4} = \tfrac{1}{4}\left(g_{\mu_1\mu_2}g_{\mu_3\mu_4} + g_{\mu_1\mu_3}g_{\mu_2\mu_4} + g_{\mu_1\mu_4}g_{\mu_2\mu_3}\right), \tag{4.11}$$

$$
\begin{aligned}
G(g)_{\mu_1\mu_2\mu_3\mu_4\mu_5\mu_6} = \tfrac{1}{8}\Big[&+ g_{\mu_1\mu_2}g_{\mu_3\mu_4}g_{\mu_5\mu_6} + g_{\mu_1\mu_2}g_{\mu_3\mu_5}g_{\mu_4\mu_6} + g_{\mu_1\mu_2}g_{\mu_3\mu_6}g_{\mu_4\mu_5} \\
&+ g_{\mu_1\mu_3}g_{\mu_2\mu_4}g_{\mu_5\mu_6} + g_{\mu_1\mu_3}g_{\mu_2\mu_5}g_{\mu_4\mu_6} + g_{\mu_1\mu_3}g_{\mu_2\mu_6}g_{\mu_4\mu_5} \\
&+ g_{\mu_1\mu_4}g_{\mu_2\mu_3}g_{\mu_5\mu_6} + g_{\mu_1\mu_4}g_{\mu_2\mu_5}g_{\mu_3\mu_6} + g_{\mu_1\mu_4}g_{\mu_2\mu_6}g_{\mu_3\mu_5} \\
&+ g_{\mu_1\mu_5}g_{\mu_2\mu_3}g_{\mu_4\mu_6} + g_{\mu_1\mu_5}g_{\mu_2\mu_4}g_{\mu_3\mu_6} + g_{\mu_1\mu_5}g_{\mu_2\mu_6}g_{\mu_3\mu_4} \\
&+ g_{\mu_1\mu_6}g_{\mu_2\mu_3}g_{\mu_4\mu_5} + g_{\mu_1\mu_6}g_{\mu_2\mu_4}g_{\mu_3\mu_5} + g_{\mu_1\mu_6}g_{\mu_2\mu_5}g_{\mu_3\mu_4}\Big]\,.
\end{aligned} \tag{4.12}
$$

Keeping the same order already obtained in the first step, we get after the contactions:

Contribution of f_1 variable: w (no contraction since $p=0$).

Contribution of f_2 variables:

$$
\begin{aligned}
-\tfrac{1}{2}g^{\mu\nu}g_{\rho\sigma}(\partial_\mu\partial_\nu g^{\rho\sigma})\, u\otimes u - g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma})\, u\otimes\partial_\mu u - \tfrac{d}{2}g^{\mu\nu}\, u\otimes\partial_\mu\partial_\nu u \\
- \tfrac{1}{2}g_{\rho\sigma}(\partial_\mu g^{\rho\sigma})\, v^\mu\otimes u - \tfrac{d}{2}\, v^\mu\otimes\partial_\mu u - \tfrac{1}{2}g_{\mu\nu}\, v^\mu\otimes v^\nu - u\otimes\partial_\mu v^\mu.
\end{aligned}
$$

Contribution of f_3 variables:

$$
\begin{aligned}
&\Big[\tfrac{1}{2}g^{\mu\nu}g_{\rho\sigma}g_{\alpha\beta}(\partial_\mu g^{\rho\sigma})(\partial_\nu g^{\alpha\beta}) + g^{\mu\nu}g_{\rho\sigma}g_{\alpha\beta}(\partial_\mu g^{\rho\alpha})(\partial_\nu g^{\sigma\beta})\Big]\, u\otimes u\otimes u\\
&+ \tfrac{d+2}{2}g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma})\, u\otimes u\otimes \partial_\mu u + \tfrac{d+2}{2}g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma})\, u\otimes \partial_\mu u\otimes u + \tfrac{d(d+2)}{2}g^{\mu\nu}\, u\otimes \partial_\mu u\otimes \partial_\nu u\\
&+ \tfrac{1}{2}g_{\rho\sigma}(\partial_\mu g^{\rho\sigma})\, v^\mu\otimes u\otimes u + g_{\mu\nu}(\partial_\rho g^{\rho\nu})\, v^\mu\otimes u\otimes u + \tfrac{d+2}{2}\, v^\mu\otimes u\otimes \partial_\mu u\\
&+ \tfrac{1}{2}g_{\rho\sigma}(\partial_\mu g^{\rho\sigma})\, u\otimes u\otimes v^\mu + g_{\mu\nu}(\partial_\rho g^{\rho\nu})\, u\otimes u\otimes v^\mu + \tfrac{d+2}{2}\, u\otimes \partial_\mu u\otimes v^\mu\\
&+ \tfrac{1}{2}g_{\rho\sigma}(\partial_\mu g^{\rho\sigma})\, u\otimes v^\mu\otimes u + g_{\mu\nu}(\partial_\rho g^{\rho\nu})\, u\otimes v^\mu\otimes u + \tfrac{d+2}{2}\, u\otimes v^\mu\otimes \partial_\mu u\\
&+ \Big[g_{\rho\sigma}(\partial_\mu g^{\mu\nu})(\partial_\nu g^{\rho\sigma}) + 2g_{\rho\sigma}(\partial_\mu g^{\nu\rho})(\partial_\nu g^{\mu\sigma})\Big]u\otimes u\otimes u + (d+2)(\partial_\nu g^{\mu\nu})\, u\otimes u\otimes \partial_\mu u\\
&+ [g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma}) + 2(\partial_\nu g^{\mu\nu})]\, u\otimes \partial_\mu u\otimes u + (d+2)g^{\mu\nu}\, u\otimes \partial_\mu u\otimes \partial_\nu u\\
&+ [g^{\mu\nu}g_{\rho\sigma}(\partial_\mu\partial_\nu g^{\rho\sigma}) + 2(\partial_\mu\partial_\nu g^{\mu\nu})]\, u\otimes u\otimes u + [g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma}) + 2(\partial_\nu g^{\mu\nu})]\, u\otimes u\otimes \partial_\mu u\\
&+ [g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma}) + 2(\partial_\nu g^{\mu\nu})]\, u\otimes u\otimes \partial_\mu u + (d+2)g^{\mu\nu}\, u\otimes u\otimes \partial_\mu\partial_\nu u.
\end{aligned}
$$

which, once collected, gives

$$
\begin{aligned}
&\Big[g^{\mu\nu}g_{\rho\sigma}(\partial_\mu\partial_\nu g^{\rho\sigma}) + 2(\partial_\mu\partial_\nu g^{\mu\nu}) + g_{\rho\sigma}(\partial_\mu g^{\mu\nu})(\partial_\nu g^{\rho\sigma}) + 2g_{\rho\sigma}(\partial_\mu g^{\nu\rho})(\partial_\nu g^{\mu\sigma})\\
&\qquad \tfrac{1}{2}g^{\mu\nu}g_{\rho\sigma}g_{\alpha\beta}(\partial_\mu g^{\rho\sigma})(\partial_\nu g^{\alpha\beta}) + g^{\mu\nu}g_{\rho\sigma}g_{\alpha\beta}(\partial_\mu g^{\rho\alpha})(\partial_\nu g^{\sigma\beta})\Big]\, u\otimes u\otimes u\\
&+ (d+6)\Big[\tfrac{1}{2}g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma}) + (\partial_\nu g^{\mu\nu})\Big]\, u\otimes u\otimes \partial_\mu u\\
&+ \Big[\tfrac{d+4}{2}g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma}) + 2(\partial_\nu g^{\mu\nu})\Big]\, u\otimes \partial_\mu u\otimes u\\
&+ \tfrac{(d+2)^2}{2}g^{\mu\nu}\, u\otimes \partial_\mu u\otimes \partial_\nu u + (d+2)g^{\mu\nu}\, u\otimes u\otimes \partial_\mu\partial_\nu u\\
&+ \Big[\tfrac{1}{2}g_{\rho\sigma}(\partial_\mu g^{\rho\sigma}) + g_{\mu\nu}(\partial_\rho g^{\rho\nu})\Big](v^\mu\otimes u\otimes u + u\otimes v^\mu\otimes u + u\otimes u\otimes v^\mu)\\
&+ \tfrac{d+2}{2}(v^\mu\otimes u\otimes \partial_\mu u + u\otimes \partial_\mu u\otimes v^\mu + u\otimes v^\mu\otimes \partial_\mu u)
\end{aligned}
$$

Contribution of f_4 variables: We use the following symmetry: in previous three terms of f_4, one goes from the first to the second right terms by the change $(\mu_2,\mu_3,\mu_4)\to(\mu_3,\mu_4,\mu_2)$ and from the second to the third terms via $(\mu,\nu)\to(\nu,\mu)$ and $(\mu_1,\mu_2)\to(\mu_2,\mu_1)$. So after the contraction of the first term and using that symmetry (which explains the factors 3 and 2), we get

$$
\begin{aligned}
&3\Big[-\tfrac{1}{2}g^{\mu\nu}g_{\rho\sigma}g_{\alpha\beta}(\partial_\mu g^{\rho\sigma})(\partial_\nu g^{\alpha\beta}) - g^{\mu\nu}g_{\rho\sigma}g_{\alpha\beta}(\partial_\mu g^{\rho\alpha})(\partial_\nu g^{\sigma\beta}) - 2g_{\rho\sigma}(\partial_\mu g^{\mu\nu})(\partial_\nu g^{\rho\sigma})\\
&\qquad - 2g_{\rho\sigma}(\partial_\mu g^{\mu\rho})(\partial_\nu g^{\nu\sigma}) - 2g_{\rho\sigma}(\partial_\mu g^{\nu\rho})(\partial_\nu g^{\mu\sigma})\Big]\, u\otimes u\otimes u\otimes u\\
&- (d+4)\Big[(\partial_\mu g^{\mu\nu}) + \tfrac{1}{2}g^{\mu\nu}g_{\rho\sigma}(\partial_\mu g^{\rho\sigma})\Big]\Big(3\, u\otimes u\otimes u\otimes \partial_\nu u\\
&\qquad\qquad + 2\, u\otimes u\otimes \partial_\nu u\otimes u + u\otimes \partial_\nu u\otimes u\otimes u\Big)\\
&- \tfrac{1}{2}(d+4)(d+2)g^{\mu\nu}\Big(2\, u\otimes u\otimes \partial_\mu u\otimes \partial_\nu u + u\otimes \partial_\mu u\otimes u\otimes \partial_\nu u\Big).
\end{aligned}
$$

It worth to mention that all results of this section 4.1 are valid in arbitrary dimension d of the manifold.

4.2. Application of operators $I_{d/2+p,k}$

We can now compute in (4.4) the application of $I_{d/2+p,k}$ on each previous $G(g)_{\mu_1\dots\mu_{2p}}\,\mathbb{B}_k^{\mu_1\cdots\mu_{2p}}$. We restrict to even dimension $d=2m$ since we will prove in Section 5.2 that it is impossible

to get explicit formulae when d is odd (explicit in the sense that we do want to avoid ending with formulae like (1.5)).

Lemma 2.6 tells us that we have only to apply the four operators given by (3.10) for $k = 1, 2, 3, 4$:

$$I_{m+k-1,k}(r_0, \dots, r_k) = \tfrac{(-1)^k}{(m-1)(m)\cdots(m+k-2)} \sum_{i=0}^{k} \Big[\prod_{\substack{j=0\\ j\neq i}}^{k} (r_i - r_j)^{-1} \Big] r_i^{-(m-1)}, \qquad \text{when } m \neq 1,$$

$$I_{k,k}(r_0, \dots, r_k) = \tfrac{(-1)^{k+1}}{(k-1)!} \sum_{i=0}^{k} \Big[\prod_{\substack{j=0\\ j\neq i}}^{k} (r_i - r_j)^{-1} \Big] r_i^{-1} \log r_i\,, \qquad \text{when } m = 1$$

$$= \lim_{m\to 1} I_{m+k-1,k}(r_0, \dots, r_k) \quad \text{(see Proposition 3.1)}.$$

They are applied on the above f_k variables which have the form $A_1 \otimes \cdots \otimes A_k$ where each A_i is equal to u, v^μ, w or their (at most second order) derivatives. Thus we can apply Lemma 4.1 since, at most, only two A_i (relabeled indistinctly B_1, B_2) are different from u. This method generates only four cases modulo $B_1 \leftrightarrow B_2$:
Case 0: only one variable, namely w.
Case 1: $B_1 = B_2 = u$.
Case 2: $(B_1 = \partial_\mu u, B_2 = u)$, $(B_1 = \partial_\mu\partial_\nu u, B_2 = u)$, $(B_1 = v^\mu, B_2 = u)$, $(B_1 = \partial_\mu v^\mu, B_2 = u)$.
Case 3: $(B_1 = v^\mu, B_2 = v^\nu)$, $(B_1 = v^\mu, B_2 = \partial_\mu u)$, $(B_1 = \partial_\mu u, B_2 = \partial_\nu u)$.

We use the shortcut

$$J_{m+k-1,k}[A_1 \otimes \cdots \otimes A_k] := \operatorname{tr}(\mathbf{m} \circ I_{m+k-1,k}[\mathbb{1} \otimes A_1 \otimes A_2 \otimes \cdots \otimes A_k]).$$

We first give two examples of such computations of J. The first one corresponds to Case 0 and is given by the variable w in f_1. Its contribution to a_1 is:

$$J_{m,1}[w] = \operatorname{tr}(\mathbf{m} \circ I_{m,1}(R_0(u), R_1(u))[\mathbb{1} \otimes w]) = \sum_{r_0,r_1} I_{m,1}(r_0, r_1) \operatorname{tr}(E_0 w E_1)$$
$$= \sum_{r_0} I_{m,1}(r_0, r_0) \operatorname{tr}(E_0 w) = \operatorname{tr}(u^{-m} w)$$

since $I_{m,1}(r_0, r_0) = r_0^{-m}$ by (3.2).
Our second example comes from Case 3 and is given by the variable $-\frac{1}{2} g_{\mu\nu}\, v^\mu \otimes v^\nu$ in f_2: we have

$$J_{m+1,2}[v^\mu \otimes v^\nu] = \operatorname{tr}(\mathbf{m} \circ I_{m+1,2}(R_0(u), R_1(u), R_2(u))[\mathbb{1} \otimes v^\mu \otimes v^\nu])$$
$$= \sum_{r_0,r_1,r_2} I_{m+1,2}(r_0, r_1, r_2) \operatorname{tr}(E_0 v^\mu E_1 v^\nu E_2) = \sum_{r_0,r_1} I_{m+1,2}(r_0, r_1, r_0) \operatorname{tr}(E_0 v^\mu E_1 v^\nu).$$

Thus, using Corollary 4.2 and (A.3), its contribution to a_1 is

$$-\tfrac{1}{2} g_{\mu\nu} J_{m+1,2}[v^\mu \otimes v^\nu] = -\tfrac{g_{\mu\nu}}{2} \sum_{r_0,r_1} \tfrac{1}{2}[I_{m+1,2}(r_0, r_1, r_0) + I_{m+1,2}(r_1, r_0, r_1)] \operatorname{tr}(E_0 v^\mu E_1 v^\nu) \quad (4.13)$$
$$= -\tfrac{1}{2} g_{\mu\nu} \sum_{r_0,r_1} \tfrac{1}{2m} \sum_{\ell=0}^{m-1} r_0^{-\ell-1}\, r_1^{\ell-m} \operatorname{tr}(E_0 v^\mu E_1 v^\nu)$$
$$= -\tfrac{1}{4m}\, g_{\mu\nu} \sum_{\ell=0}^{m-1} \operatorname{tr}(u^{-\ell-1} v^\mu u^{\ell-m} v^\nu).$$

We now consider all contributions.

Case 1:

Thanks to (3.2)

$$J_{m+k-1,k}[\underbrace{u\otimes\cdots\otimes u}_{k}] = \tfrac{1}{k!}\,\mathrm{tr}(u^{-m+1})$$

and we get

$$\begin{aligned}
&-\tfrac{1}{2}g^{\mu\nu}g_{\rho\sigma}(\partial_\mu\partial_\nu g^{\rho\sigma})\,J_{m+1,2}[u\otimes u]\\
&+\Big[g^{\mu\nu}g_{\rho\sigma}(\partial_\mu\partial_\nu g^{\rho\sigma})+2(\partial_\mu\partial_\nu g^{\mu\nu})+g_{\rho\sigma}(\partial_\mu g^{\mu\nu})(\partial_\nu g^{\rho\sigma})+2g_{\rho\sigma}(\partial_\mu g^{\nu\rho})(\partial_\nu g^{\mu\sigma})\\
&\qquad\tfrac{1}{2}g^{\mu\nu}g_{\rho\sigma}g_{\alpha\beta}(\partial_\mu g^{\rho\sigma})(\partial_\nu g^{\alpha\beta})+g^{\mu\nu}g_{\rho\sigma}g_{\alpha\beta}(\partial_\mu g^{\rho\alpha})(\partial_\nu g^{\sigma\beta})\Big]\,J_{m+2,3}[u\otimes u\otimes u]\\
&+3\Big[-\tfrac{1}{2}g^{\mu\nu}g_{\rho\sigma}g_{\alpha\beta}(\partial_\mu g^{\rho\sigma})(\partial_\nu g^{\alpha\beta})-g^{\mu\nu}g_{\rho\sigma}g_{\alpha\beta}(\partial_\mu g^{\rho\alpha})(\partial_\nu g^{\sigma\beta})-2g_{\rho\sigma}(\partial_\mu g^{\mu\nu})(\partial_\nu g^{\rho\sigma})\\
&\qquad-2g_{\rho\sigma}(\partial_\mu g^{\mu\rho})(\partial_\nu g^{\nu\sigma})-2g_{\rho\sigma}(\partial_\mu g^{\nu\rho})(\partial_\nu g^{\mu\sigma})\Big]\,J_{m+3,4}[u\otimes u\otimes u\otimes u]\\
&\qquad=\alpha\,\mathrm{tr}(u^{-m+1})
\end{aligned}$$

where

$$\begin{aligned}
\alpha :=\ &\tfrac{1}{3}(\partial_\mu\partial_\nu g^{\mu\nu})-\tfrac{1}{12}g^{\mu\nu}g_{\rho\sigma}(\partial_\mu\partial_\nu g^{\rho\sigma})+\tfrac{1}{48}g^{\mu\nu}g_{\rho\sigma}g_{\alpha\beta}(\partial_\mu g^{\rho\sigma})(\partial_\nu g^{\alpha\beta})\\
&+\tfrac{1}{24}g^{\mu\nu}g_{\rho\sigma}g_{\alpha\beta}(\partial_\mu g^{\rho\alpha})(\partial_\nu g^{\sigma\beta})-\tfrac{1}{12}g_{\rho\sigma}(\partial_\mu g^{\mu\nu})(\partial_\nu g^{\rho\sigma})\\
&+\tfrac{1}{12}g_{\rho\sigma}(\partial_\mu g^{\nu\rho})(\partial_\nu g^{\mu\sigma})-\tfrac{1}{4}g_{\rho\sigma}(\partial_\mu g^{\mu\rho})(\partial_\nu g^{\nu\sigma}).
\end{aligned}\tag{4.14}$$

Case 2:

$(B_1=\partial_\mu u, B_2=u)$ generating terms in $\mathrm{tr}(u^{-m}\partial_\mu u)$ with coefficient

$$\begin{aligned}
&-\tfrac{1}{2}g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma})+\tfrac{(2m+6)}{3!}\Big[\tfrac{1}{2}g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma})+(\partial_\nu g^{\mu\nu})\Big]+\tfrac{1}{3!}\Big[\tfrac{2m+4}{2}g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma})+2(\partial_\nu g^{\mu\nu})\Big]\\
&-\tfrac{6(2m+4)}{4!}\Big[(\partial_\nu g^{\mu\nu})+\tfrac{1}{2}g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma})\Big]\\
&\qquad=\tfrac{m-2}{6}\Big[\tfrac{1}{2}g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma})-(\partial_\nu g^{\mu\nu})\Big]
\end{aligned}$$

$(B_1=\partial_\mu\partial_\nu u, B_2=u)$ generating terms in $\mathrm{tr}(u^{-m}\partial_\mu\partial_\nu u)$ with coefficient

$$-\tfrac{2m}{2}g^{\mu\nu}\tfrac{1}{2!}+(2m+2)g^{\mu\nu}\tfrac{1}{3!}=-\tfrac{m-2}{6}g^{\mu\nu}$$

$(B_1=v^\mu, B_2=u)$ generating terms in $\mathrm{tr}(u^{-m}v^\mu)$ with coefficient

$$-\tfrac{1}{2}\tfrac{1}{2!}g_{\rho\sigma}(\partial_\mu g^{\rho\sigma})+\tfrac{3}{3!}\Big[\tfrac{1}{2}g_{\rho\sigma}(\partial_\mu g^{\rho\sigma})+g_{\mu\nu}(\partial_\rho g^{\rho\nu})\Big]=\tfrac{1}{2}g_{\mu\nu}(\partial_\rho g^{\rho\nu}).$$

$(B_1=\partial_\mu v^\mu, B_2=u)$ generating a term in $\mathrm{tr}(u^{-m}\partial_\mu v^\mu)$ with coefficient $-\frac{1}{2!}=-\frac{1}{2}$.

Case 3:

$(B_1=v^\mu, B_2=\partial_\mu u)$ generating terms in $\mathrm{tr}[E_0v^\mu E_1(\partial_\mu u)]$ with coefficient

$$\begin{aligned}
&\sum_{r_0,r_1}\Big(-mI_{m+1,2}(r_0,r_1,r_0)\\
&\qquad+\tfrac{2m+2}{2}[r_1\,I_{m+2,3}(r_0,r_1,r_1,r_0)+r_1\,I_{m+2,3}(r_1,r_1,r_0,r_1)+r_0\,I_{m+2,3}(r_0,r_0,r_1,r_0)]\Big)\\
&\qquad=\tfrac{1}{2m}\sum_{\ell=0}^{m-1}(m-2\ell)\,r_0^{-\ell-1}\,r_1^{\ell-m}
\end{aligned}$$

thanks to (A.4). So this contribution is

$$\tfrac{1}{2m}\sum_{\ell=0}^{m-1}(m-2\ell)\ \mathrm{tr}[u^{-\ell-1}v^\mu\, u^{\ell-m}(\partial_\mu u)]$$

$(B_1=\partial_\mu u, B_2=\partial_\nu u)$ generating terms in $\mathrm{tr}[E_0(\partial_\mu u)E_1(\partial_\nu u)]$ with coefficient

$$\begin{aligned}&2(m+1)^2 g^{\mu\nu} r_0\, I_{m+2,3}(r_0,r_0,r_1,r_0)\\&-2(m+2)(m+1)g^{\mu\nu}[2r_0^2 I_{m+3,4}(r_0,r_0,r_0,r_1,r_0)+r_0\,r_1\,I_{m+3,4}(r_0,r_0,r_1,r_1,r_0)]\\&=g^{\mu\nu}\,g_3(r_0,r_1)\end{aligned}$$

with the definition of g_3 in (A.5). Thanks to (A.6), this contribution is

$$\tfrac{1}{6m}g^{\mu\nu}\sum_{\ell=0}^{m-1}(m^2-2m-3\ell(m-1-\ell))\ \mathrm{tr}[u^{-\ell-1}(\partial_\mu u)u^{\ell-m}(\partial_\nu u)].$$

4.3. Main results

The recollection of all contributions (4.4) for $a_1(x)$ from Cases 0–3 is now ready for the first interesting result:

Theorem 4.3 *Assume that $P=-(u\,g^{\mu\nu}\partial_\mu\partial_\nu+v^\nu\partial_\nu+w)$ is a selfadjoint elliptic operator acting on $L^2(M,V)$ for a $2m$-dimensional boundaryless Riemannian compact manifold (M,g) and a vector bundle V over M where u,v^μ,w are local maps on M with values in M_N, with u positive and invertible. Then, its local $a_1(x)$ heat-coefficient in (1.3) for $x\in M$ is*

$$\begin{aligned}a_1=&g_{2m}\Big(\mathrm{tr}(u^{-m}w)+\alpha\,\mathrm{tr}(u^{-m+1})+\tfrac{m-2}{6}\Big[\tfrac12 g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma})-(\partial_\nu g^{\mu\nu})\Big]\mathrm{tr}(u^{-m}\partial_\mu u)\\&-\tfrac{m-2}{6}g^{\mu\nu}\,\mathrm{tr}(u^{-m}\partial_\mu\partial_\nu u)+\tfrac12 g_{\mu\nu}(\partial_\rho g^{\rho\nu})\,\mathrm{tr}(u^{-m}v^\mu)-\tfrac12\,\mathrm{tr}(u^{-m}\partial_\mu v^\mu)\\&-\tfrac{1}{4m}\sum_{\ell=0}^{m-1}g_{\mu\nu}\,\mathrm{tr}(u^{-\ell-1}v^\mu u^{\ell-m}v^\nu)+\tfrac{1}{2m}\sum_{\ell=0}^{m-1}(m-2\ell)\ \mathrm{tr}[u^{-\ell-1}v^\mu\,u^{\ell-m}(\partial_\mu u)]\\&+\sum_{\ell=0}^{m-1}\Big[\tfrac{m-2}{6}-\tfrac{\ell(m-\ell-1)}{2m}\Big]g^{\mu\nu}\,\mathrm{tr}[u^{-\ell-1}(\partial_\mu u)u^{\ell-m}(\partial_\nu u)]\Big)\end{aligned}\tag{4.15}$$

where α is given in (4.14).

Since the operator P is not written in terms of objects which have simple (homogeneous) transformations by change of coordinates and gauge transformation, this result does not make apparent any explicit Riemannian or gauge invariant expressions. This is why we have not used normal coordinates until now. Nevertheless, from Lemma A.5, one can deduce after a long computation:

Lemma 4.4 *Under a gauge transformation, $a_1(x)$ given by (4.15) is gauge invariant.*

As shown in A.4, with the help of a gauge connection A_μ, one can change the variables (u,v^μ,w) to variables (u,p^μ,q) well adapted to changes of coordinates and gauge transformations (see (A.12) and (A.13)). For $u^{\mu\nu}=g^{\mu\nu}u$, (A.14) and (A.15) becomes

$$v^\mu=\Big[-\tfrac12 g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma})+\partial_\nu g^{\mu\nu}\Big]u+g^{\mu\nu}(\partial_\nu u)+g^{\mu\nu}(uA_\nu+A_\nu u)+p^\mu\tag{4.16}$$

$$\begin{aligned}w=&\Big[-\tfrac12 g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma})+\partial_\nu g^{\mu\nu}\Big]uA_\mu+g^{\mu\nu}(\partial_\nu u)A_\mu+g^{\mu\nu}u(\partial_\mu A_\nu)\\&+g^{\mu\nu}A_\mu uA_\nu+p^\mu A_\mu+q.\end{aligned}\tag{4.17}$$

Relations (4.16) and (4.17) can be injected into (4.15) to get an explicitly diffeomorphism and gauge invariant expression. In order to present the result of this straightforward computation, let us introduce the following notations.

Given the Christoffel symbols $\Gamma^\rho_{\mu\nu} := \frac{1}{2}g^{\rho\sigma}(\partial_\mu g_{\sigma\nu} + \partial_\nu g_{\sigma\mu} - \partial_\sigma g_{\mu\nu})$, the Riemann curvature tensor $R^\alpha_{\beta\mu\nu} := \partial_\mu\Gamma^\alpha_{\beta\nu} - \partial_\nu\Gamma^\alpha_{\beta\mu} + \Gamma^\alpha_{\mu\rho}\Gamma^\rho_{\beta\nu} - \Gamma^\alpha_{\nu\rho}\Gamma^\rho_{\beta\mu}$, and the Ricci tensor $R_{\mu\nu} := R^\rho_{\mu\rho\nu}$, the scalar curvature $R := g^{\mu\nu}R_{\mu\nu}$ computed in terms of the derivatives of the inverse metric is

$$\begin{aligned} R = g^{\mu\nu}g_{\rho\sigma}(\partial_\mu\partial_\nu g^{\rho\sigma}) - (\partial_\mu\partial_\nu g^{\mu\nu}) + g_{\rho\sigma}(\partial_\mu g^{\mu\nu})(\partial_\nu g^{\rho\sigma}) + \tfrac{1}{2}g_{\rho\sigma}(\partial_\mu g^{\nu\rho})(\partial_\nu g^{\mu\sigma}) \\ - \tfrac{1}{4}g^{\mu\nu}g_{\rho\sigma}g_{\alpha\beta}(\partial_\mu g^{\rho\sigma})(\partial_\nu g^{\alpha\beta}) - \tfrac{5}{4}g^{\mu\nu}g_{\rho\sigma}g_{\alpha\beta}(\partial_\mu g^{\rho\alpha})(\partial_\nu g^{\sigma\beta}), \end{aligned} \tag{4.18}$$

and one has

$$g^{\mu\nu}\Gamma^\rho_{\mu\nu} = \tfrac{1}{2}g^{\rho\sigma}g_{\alpha\beta}(\partial_\sigma g^{\alpha\beta}) - \partial_\sigma g^{\rho\sigma}, \qquad \Gamma^\sigma_{\sigma\rho} = -\tfrac{1}{2}g_{\alpha\beta}(\partial_\rho g^{\alpha\beta}).$$

Let ∇_μ be the (gauge) covariant derivative on V (and its related bundles):

$$\nabla_\mu s := \partial_\mu s + A_\mu s \quad \text{for any section } s \text{ of } V.$$

From (A.13), u, p^μ and q are sections of the endomorphism vector bundle $\mathrm{End}(V) = V^* \otimes V$ (while v^μ and w are not), so that $\nabla_\mu u = \partial_\mu u + [A_\mu, u]$ (and the same for p^μ and q). We now define $\widehat{\nabla}_\mu$, which combines ∇_μ and the linear connection induced by the metric g:

$$\begin{aligned} \widehat{\nabla}_\mu u := \partial_\mu u + [A_\mu, u] = \nabla_\mu u, \qquad \widehat{\nabla}_\mu p^\rho := \partial_\mu p^\rho + [A_\mu, p^\rho] + \Gamma^\rho_{\mu\nu}p^\nu = \nabla_\mu p^\rho + \Gamma^\rho_{\mu\nu}p^\nu \\ \widehat{\nabla}_\mu\widehat{\nabla}_\nu u := \partial_\mu\widehat{\nabla}_\nu u + [A_\mu, \widehat{\nabla}_\nu u] - \Gamma^\rho_{\mu\nu}\widehat{\nabla}_\rho u = \partial_\mu\nabla_\nu u + [A_\mu, \nabla_\nu u] - \Gamma^\rho_{\mu\nu}\nabla_\rho u\,, \end{aligned}$$

so that, if $\Delta^{\widehat{\nabla}} := g^{\mu\nu}\,\widehat{\nabla}_\mu\widehat{\nabla}_\nu$ is the connection Laplacian

$$\begin{aligned} \Delta^{\widehat{\nabla}}\, u &= g^{\mu\nu}\nabla_\mu\nabla_\nu u - \left[\tfrac{1}{2}g^{\mu\nu}g_{\alpha\beta}(\partial_\mu g^{\alpha\beta}) - \partial_\mu g^{\mu\nu}\right]\nabla_\nu u, \\ \widehat{\nabla}_\mu p^\mu &= \nabla_\mu p^\mu - \tfrac{1}{2}g_{\alpha\beta}(\partial_\mu g^{\alpha\beta})p^\mu. \end{aligned}$$

Any relation involving u, p^μ, q, g and $\widehat{\nabla}_\mu$ inherits the homogeneous transformations by changes of coordinates and gauge transformations of these objects.

Let us state now the result of the computation of $a_1(x)$ in terms of (u, p^μ, q):

Theorem 4.5 *Assume that $P = -(|g|^{-1/2}\nabla_\mu|g|^{1/2}g^{\mu\nu}u\nabla_\nu + p^\mu\nabla_\mu + q)$ is a selfadjoint elliptic operator acting on $L^2(M,V)$ for a $2m$-dimensional boundaryless Riemannian compact manifold (M,g) and a vector bundle V over M where u, p^μ, q are sections of endomorphisms on V with u positive and invertible. Then, its local $a_1(x)$ heat-coefficient in (1.3) for $x \in M$ is*

$$\begin{aligned} a_1 =& g_{2m}\Big(\tfrac{1}{6}R\,\mathrm{tr}[u^{1-m}] + \mathrm{tr}[u^{-m}q] - \tfrac{m+1}{6}\,\mathrm{tr}[u^{-m}\Delta^{\widehat{\nabla}}u] - \tfrac{1}{2}\,\mathrm{tr}[u^{-m}\widehat{\nabla}_\mu p^\mu] \\ &+ \sum_{\ell=0}^{m-1}\left[\tfrac{2m^2-4m+3}{12m} - \tfrac{\ell(m-\ell-1)}{2m}\right]g^{\mu\nu}\,\mathrm{tr}[u^{-\ell-1}(\widehat{\nabla}_\mu u)u^{\ell-m}(\widehat{\nabla}_\nu u)] \\ &+ \tfrac{1}{2m}\sum_{\ell=0}^{m-1}(m-2\ell-1)\,\mathrm{tr}[u^{-\ell-1}p^\mu u^{\ell-m}(\widehat{\nabla}_\mu u)] - \tfrac{1}{4m}\sum_{\ell=0}^{m-1}g_{\mu\nu}\,\mathrm{tr}[u^{-\ell-1}p^\mu u^{\ell-m}p^\nu]\Big) \end{aligned} \tag{4.19}$$

where $g_{2m} = \frac{\sqrt{|g|}}{4^m\,\pi^m}$.

Proof This can be checked by an expansion of the RHS of (4.19). A more subtle method goes using normal coordinates in (4.15), (4.16), (4.17), knowing that $a_1(x)$ is a scalar and $(u,\, p^\mu,\, q)$ are well adapted to change of coordinates. The coefficients in the sum of the second line of this expression have been symmetrized $\ell \leftrightarrow (m-\ell-1)$ using the trace property and the change of variable $\ell \mapsto m-\ell-1$. ■

Corollary 4.6 *The previous formula can be written in a more compact way as*

$$\begin{aligned} a_1 =& g_{2m}\Big(\tfrac{1}{6}R\,\mathrm{tr}[u^{1-m}] + \mathrm{tr}[u^{-m}q] - \tfrac{m+1}{6}\,\mathrm{tr}[u^{-m}\Delta^{\widehat{\nabla}}u] - \tfrac{1}{2}\,\mathrm{tr}[u^{-m}\widehat{\nabla}_\mu p^\mu] \\ &+ \tfrac{1}{4m}\sum_{\ell=0}^{m-1} g^{\mu\nu}\,\mathrm{tr}[u^{-\ell-1}[(2\ell-1)\widehat{\nabla}_\mu u - p_\mu]u^{\ell-m}[(2\ell-1)\widehat{\nabla}_\nu u + p_\nu]] \\ &+ \tfrac{1}{2m}\sum_{\ell=0}^{m-1} g^{\mu\nu}\,\mathrm{tr}[u(\widehat{\nabla}_\mu u^{-\ell-1})u(\widehat{\nabla}_\nu u^{\ell-m})] \\ &- \tfrac{m^2-2m+3}{3m}\sum_{\ell=0}^{m-1} g^{\mu\nu}\,\mathrm{tr}[u^{-\ell-1}(\widehat{\nabla}_\mu u)u^{\ell-m}(\widehat{\nabla}_\nu u)]\Big) \end{aligned} \tag{4.20}$$

where $p_\mu = g_{\mu\nu}p^\nu$.

Proof This relation can be obtained by expanding the second and third lines of (4.20) using the combinatorial equality

$$\sum_{\ell=0}^{m-1} g^{\mu\nu}\,\mathrm{tr}[u(\partial_\mu u^{-\ell-1})u(\partial_\nu u^{\ell-m})] = \sum_{\ell=0}^{m-1}\Big[m+\ell(m-\ell-1)\Big]\,g^{\mu\nu}\,\mathrm{tr}[u^{-\ell-1}(\partial_\mu u)u^{\ell-m}(\partial_\nu u)]$$

that is a tedious computation. ■

The above formula (4.20) is not the unique way to write (4.19). Some variations are possible using for instance the relations

$$\begin{aligned} g^{\mu\nu}\,\mathrm{tr}[u(\partial_\mu\partial_\nu u^{-m})] &= -m\,g^{\mu\nu}\,\mathrm{tr}[u^{-m}(\partial_\mu\partial_\nu u)] + (m+1)\sum_{\ell=0}^{m-1} g^{\mu\nu}\,\mathrm{tr}[u^{-\ell-1}(\partial_\mu u)u^{\ell-m}(\partial_\nu u)], \\ \sum_{\ell=0}^{m-1} g^{\mu\nu}\,\mathrm{tr}[u(\partial_\mu u^{-\ell})(\partial_\nu u^{\ell-m})] &= \sum_{\ell=0}^{m-1}\Big[\tfrac{m-1}{2}+\ell(m-\ell-1)\Big]\,g^{\mu\nu}\,\mathrm{tr}[u^{-\ell-1}(\partial_\mu u)u^{\ell-m}(\partial_\nu u)], \\ g^{\mu\nu}\,\mathrm{tr}[\partial_\mu(u^{-m}\partial_\nu u)] &= g^{\mu\nu}\,\mathrm{tr}[u^{-m}(\partial_\mu\partial_\nu u)] - \sum_{\ell=0}^{m-1} g^{\mu\nu}\,\mathrm{tr}[u^{-\ell-1}(\partial_\mu u)u^{\ell-m}(\partial_\nu u)], \end{aligned}$$

which make all appear the expression $g^{\mu\nu}\,\mathrm{tr}[u^{-\ell-1}(\partial_\mu u)u^{\ell-m}(\partial_\nu u)]$ in (4.19).

Corollary 4.7 *When M has dimension 4, the last two terms of (4.20) compensate and the formula simplifies as*

$$\begin{aligned} a_1 =& \tfrac{|g|^{1/2}}{16\,\pi^2}\Big(\tfrac{1}{6}R\,\mathrm{tr}[u^{-1}] + \mathrm{tr}[u^{-2}q] - \tfrac{1}{2}g^{\mu\nu}\,\mathrm{tr}[u^{-2}\widehat{\nabla}_\mu\widehat{\nabla}_\nu u] - \tfrac{1}{2}\,\mathrm{tr}[u^{-2}\widehat{\nabla}_\mu p^\mu] \\ &+ \tfrac{1}{4}g^{\mu\nu}\,\mathrm{tr}[u^{-2}(\widehat{\nabla}_\mu u - p_\mu)u^{-1}(\widehat{\nabla}_\nu u + p_\nu)]\Big). \end{aligned} \tag{4.21}$$

Remark 4.8 For the computation of $a_r(x)$ with $r \geq 2$, directly in terms of variables (u, p^μ, q), the strategy is to use normal coordinates from the very beginning, which simplifies the computation of terms $\mathbb{B}_k^{\mu_1\cdots\mu_{2p}}$ of (4.4). Then an equivalent result to Theorem 4.3 would be obtained, but only valid in normal coordinates. Thus, by the change of variables (4.16), (4.17), a final result as Theorem 4.5 could be calculated. □

Remark 4.9 In the present method, the factor $\frac{1}{6}R$ is explicitly and straightforwardly computed from the metric entering $u^{\mu\nu} = g^{\mu\nu}u$, as in [3] for instance. Many methods introduce R using diffeomorphism invariance and compute the coefficient $\frac{1}{6}$ using some "conformal perturbation" of P (see [24, Section 3.3]). □

4.4. Case of scalar symbol: $u(x) = f(x)\,\mathbb{1}_N$

Let us consider now the specific case $u(x) = f(x)\,\mathbb{1}_N$, where f is a nowhere vanishing positive function. Then (4.16) simplifies to

$$v^\mu = [-\tfrac{1}{2}g^{\mu\nu}g_{\rho\sigma}(\partial_\nu g^{\rho\sigma}) + \partial_\nu g^{\mu\nu}]f\,\mathbb{1}_N + g^{\mu\nu}(\partial_\nu f)\,\mathbb{1}_N + 2f\,g^{\mu\nu}A_\nu + p^\mu$$

and we can always find A_μ such that $p^\mu = 0$:

$$A_\mu = \tfrac{1}{2}\Big(g_{\mu\nu}f^{-1}v^\nu + [\tfrac{1}{2}g_{\rho\sigma}(\partial_\mu g^{\rho\sigma}) - g_{\mu\nu}(\partial_\rho g^{\rho\nu}) - f^{-1}(\partial_\mu f)]\,\mathbb{1}_N\Big).$$

One can check, using (A.8), that A_μ satisfies the correct gauge transformations. This means that P can be written as

$$P = -(|g|^{-1/2}\nabla_\mu|g|^{1/2}g^{\mu\nu}f\nabla_\nu + q)$$

where the only matrix-dependencies are in q and A_μ.

Since u is in the center, $\nabla_\mu u = (\partial_\mu f)\,\mathbb{1}_N$ and (4.19) simplifies as

$$\begin{aligned} a_1 = g_{2m}f^{-m}[\tfrac{N}{6}\,f\,R + \mathrm{tr}[q] - \tfrac{m+1}{6}Ng^{\mu\nu}(\partial_\mu\partial_\nu f) + \tfrac{m+1}{6}Ng^{\mu\nu}\Gamma^\rho_{\mu\nu}(\partial_\rho f) \\ + \tfrac{m^2-m+1}{12}Ng^{\mu\nu}f^{-1}(\partial_\mu f)(\partial_\nu f)] \end{aligned}$$

in which A_μ does not appears. Now, if f is constant, we get the well-known result (see [24, Section 3.3]):

$$a_1 = g_{2m}f^{-m}\Big(\tfrac{N}{6}\,R + \mathrm{tr}[q]\Big).$$

5. About the method

5.1. Existence

For the operator P given in (1.1), the method used here assumes only the existence of asymptotics (1.3). This is the case when P is elliptic and selfadjoint.
Selfadjointness of P on $L^2(M, V)$ is not really a restriction since we remark that given an arbitrary family of $u^{\mu\nu}$ satisfying (1.2), skewadjoint matrices $\tilde{v}^\mu$ and a selfadjoint matrix $\tilde{w}$, we get a formal selfadjoint elliptic operator P defined by (1.1) where

$$\begin{aligned} v^\mu &= \tilde{v}^\mu + (\partial_\nu \log|g|^{1/2})\,u^{\mu\nu} + \partial_\nu u^{\mu\nu}, \\ w &= \tilde{w} + \tfrac{1}{2}[-\partial_\mu\tilde{v}^\mu + (\partial_\mu \log|g|^{1/2})\,\tilde{v}^\mu]. \end{aligned}$$

A crucial step in our method is to be able to compute the integral (2.18) for a general $u^{\mu\nu}$. The case $u^{\mu\nu} = g^{\mu\nu}u$ considered in Section 4 makes that integral manageable.

5.2. On explicit formulae for $u^{\mu\nu} = g^{\mu\nu}u$

For $u^{\mu\nu} = g^{\mu\nu}u$, the proposed method is a direct computational machinery. Since the method can be computerized, this could help to get a_r in Case 2 (d even and $r < d/2$). Recall the steps: 1) to expand the arguments of the initial f_k's, 2) to contract with the tensor $G(g)$, 3) to apply to the corresponding operators $I_{\alpha,k}$, 4) to collect all similar terms. Further eventual steps: 5) to change variables to (u, p^μ, q), 6) to identify (usual) Riemannian tensors and covariant derivatives (in terms of A_μ and Christoffel symbols).

Is it possible to get explicit formulae for a_r from the original ingredients (u, v^μ, w) of P? An explicit formula should look like (4.15) or (4.19). This excludes the use of spectral decomposition of u as in (1.5) which could not be recombined as

$$\sum_{\text{finite sum}} \operatorname{tr}[h_{(0)}(u)B_1 h_{(1)}(u)B_2 \cdots B_k h_{(k)}(u)]$$

where the h_i are continuous functions and the B_i are equal to u, v^μ, w or their derivatives. The obstruction to get such formula could only come from the operators $I_{\alpha,k}$ and not from the arguments B_i. Thus the matter is to understand the u-dependence of $I_{\alpha,k}$.

Let us consider $I_{\alpha,k}$ as a map $u \mapsto I_{\alpha,k}(u)$. An operator map $u \mapsto A(u) \in \mathcal{B}(\widehat{\mathcal{H}}_k)$ is called *u-factorizable* (w.r.t. the tensor product) if it can be written as

$$A(u) = \sum_{\text{finite sum}} R_0(h_{(0)}(u))\, R_1(h_{(1)}(u)) \cdots R_k(h_{(k)}(u))$$

where the $h_{(i)}$ are continuous functions on $\mathbb{R}_+^*$.

Lemma 5.1 *Let $u \mapsto A(u) = F(R_0(u), \ldots, R_k(u))$ the operator map defined by a continuous function $F : (\mathbb{R}_+^*)^{k+1} \to \mathbb{R}_+^*$. Then A is u-factorizable iff F is decomposed as*

$$F(r_0, \ldots, r_k) = \sum_{\textit{finite sum}} h_{(0)}(r_0)h_{(1)}(r_1)\cdots h_{(k)}(r_k) \tag{5.1}$$

for continuous functions $h_{(i)}$.

Proof Let λ_i be the eigenvalues of u and π_i the associated eigenprojections. If F is decomposed, then by functional calculus, one gets

$$\begin{aligned} A(u) &= \sum_{i_0,\ldots,i_k} F(\lambda_{i_0}, \ldots, \lambda_{i_k})\, R_0(\pi_{i_0}) \cdots R_k(\pi_{i_k}) \\ &= \sum_{i_0,\ldots,i_k} \sum_{\text{finite sum}} h_{(0)}(\lambda_{i_0}) \cdots h_{(k)}(\lambda_{i_k})\, R_0(\pi_{i_0}) \cdots R_k(\pi_{i_k}) \\ &= \sum_{\text{finite sum}} R_0(h_{(0)}(u)) \cdots R_k(h_{(k)}(u)). \end{aligned}$$

If A is u-factorizable, then this computation can be seen in the other way around to show that F is decomposed. ■

The general solutions (3.10) and (3.11) for the operators $I_{\alpha,k}$ are not manifestly u-factorizable because of the factors $(r_i - r_j)^{-1}$. For Case 2, Proposition 3.5 shows that $I_{\alpha,k}$ is indeed a u-factorizable operator (see also (3.15)).

The explicit expressions of the operators $I_{\alpha,k} \in \mathcal{B}(\widehat{\mathcal{H}}_k)$ don't give a definitive answer about the final formula: for instance, when applied to an argument containing some u's, the

expression can simplify a lot (see for example Case 1 of Section 4.2). Moreover, the trace and the multiplication introduce some degrees of freedom in the writing of the final expression. This leads us to consider two operators A and A' as *equivalent* when

$$\mathrm{tr} \circ \mathbf{m} \circ \kappa^* \circ A[B_1 \otimes \cdots \otimes B_k] = \mathrm{tr} \circ \mathbf{m} \circ \kappa^* \circ A'[B_1 \otimes \cdots \otimes B_k]$$

for any $B_1 \otimes \cdots \otimes B_k \in \mathcal{H}_k$. The equivalence is reminiscent of the lift from $\mathcal{B}(\mathcal{H}_k, M_N)$ to $\mathcal{B}(\widehat{\mathcal{H}_k})$ (see Remark 2.2) combined with the trace.

Lemma 5.2 *With*

$$\widetilde{I}_{\alpha,k}(r_0, \ldots, r_{k-1}) := I_{\alpha,k}(r_0, \ldots, r_{k-1}, r_0) \quad (= \lim_{r_k \to r_0} I_{\alpha,k}(r_0, \ldots, r_{k-1}, r_k)),$$

the operator $\widetilde{I}_{\alpha,k} := \widetilde{I}_{\alpha,k}(R_0(u), \ldots, R_{k-1}(u)) = I_{\alpha,k}(R_0(u), \ldots, R_{k-1}(u), R_0(u)) \in \mathcal{B}(\widehat{\mathcal{H}_k})$ *is equivalent with the original* $I_{\alpha,k}$.

Proof For any $B_1 \otimes \cdots \otimes B_k \in \mathcal{H}_k$, using previous notations, one has

$$\begin{aligned}
\mathrm{tr}(\circ \mathbf{m} \circ \kappa^* \circ I_{\alpha,k}[B_1 \otimes \cdots \otimes B_k]) &= \sum_{i_0,\ldots,i_k} I_{\alpha,k}(\lambda_{i_0}, \ldots, \lambda_{i_k}) \, \mathrm{tr}\left(\pi_{i_0} B_1 \pi_{i_1} \cdots B_k \pi_{i_k}\right) \\
&= \sum_{i_0,\ldots,i_k} I_{\alpha,k}(\lambda_{i_0}, \ldots, \lambda_{i_k}) \, \mathrm{tr}\left(\pi_{i_k} \pi_{i_0} B_1 \pi_{i_1} \cdots B_k\right) \\
&= \sum_{i_0,\ldots,i_k} I_{\alpha,k}(\lambda_{i_0}, \ldots, \lambda_{i_k}) \, \delta_{i_0,i_k} \, \mathrm{tr}\left(\pi_{i_0} B_1 \pi_{i_1} \cdots B_k\right) \\
&= \sum_{i_0,\ldots,i_{k-1}} \widetilde{I}_{\alpha,k}(\lambda_{i_0}, \ldots, \lambda_{i_{k-1}}) \, \mathrm{tr}\left(\pi_{i_0} B_1 \pi_{i_1} \cdots B_k\right) \\
&= \mathrm{tr} \circ \mathbf{m} \circ \kappa^* \circ \widetilde{I}_{\alpha,k}[B_1 \otimes \cdots \otimes B_k].
\end{aligned}$$

■

The equivalence between $\widetilde{I}_{\alpha,k}$ and $I_{\alpha,k}$ seems to be the only generic one we can consider.

We have doubts on the fact that the operators $I_{\alpha,k}$ can be always equivalent to some u-factorizable operators. For instance,

Proposition 5.3 *The contribution to* a_1 *of* (4.13) *generates always a non-explicit formula when the dimension* d *is odd, unless* u *and* v^μ *have commutation relations.*

In fact,

$$h_d(r_0^{1/2}, r_1^{1/2}) := \tfrac{1}{2}[I_{d/2+1,2}(r_0, r_1, r_0) + I_{d/2+1,2}(r_1, r_0, r_1)] = \tfrac{1}{d}(r_1 \, r_0)^{-d/2} \, \tfrac{r_0^{d/2} - r_1^{d/2}}{r_0 - r_1}$$

and we prove below that the map $h_d(x, y)$ for $(x, y) \in (\mathbb{R}_+^*)^2$ is explicit only when d is even:

Lemma 5.4 *The function* $h_d(x, y) = \sum_{finite} h_{(1)}(x) \, h_{(2)}(y)$ *with continuous functions* $h_{(i)}$ *if and only if* d *is even.*

Proof It is equivalent to show that function $d\,(xy)^d \, h_d(x, y)$ has or not such decomposition. Assume that $d = 2m$. Then we have the decomposition

$$d\,(xy)^d \, h_d(x, y) = \tfrac{x^{2m} - y^{2m}}{x^2 - y^2} = \sum_{\ell=0}^{m-1} x^{2m-2\ell-2} \, y^{2\ell}.$$

Assume now $d = 2m+1$. Then,

$$d\,(xy)^d\,h_d(x,y) = \tfrac{x^{2m+1}-y^{2m+1}}{x^2-y^2} = y^{2m}\,\tfrac{1}{x+y} + \sum_{\ell=0}^{m-1} x^{2m-1-2\ell} y^{2\ell}\,,$$

(for $m=0$ there is no sum). This expression is not decomposable since the map $(x+y)^{-1}$ is not decomposable:
Suppose we have such decomposition $(x+y)^{-1} = \sum_{\ell=1}^N h_{1,\ell}(x)\,h_{2,\ell}(y)$ for $N \in \mathbb{N}^*$. Let $(x_i,y_i)_{1\le i\le N}$ be N points in $(\mathbb{R}_+^*)^2$ and consider the $N\times N$-matrix $c_{i,j} := (x_i+y_j)^{-1}$. Then

$$\det(c) = \Big[\prod_{i,j=1}^N (x_i+y_j)\Big]^{-1} \prod_{1\le i<j\le N} (x_i-x_j)(y_i-y_j).$$

This expression shows that we can choose a family $(x_i,y_i)_{1\le i\le N}$ such that $\det(c)\neq 0$. With such a family, define the two matrices $a_{i,\ell} := h_{1,\ell}(x_i)$ and $b_{i,\ell} := h_{2,\ell}(y_i)$. Then

$$c_{i,j} = (x_i+y_j)^{-1} = \sum_{\ell=1}^N h_{1,\ell}(x)\,h_{2,\ell}(y_j) = \sum_{\ell=1}^N a_{i,\ell}\,b_{j,\ell}$$

so that, in matrix notation, $c = a\cdot {}^t b$, which implies that $\det(a)\neq 0$ and $\det(b)\neq 0$. From $(x+y_j)^{-1} = \sum_{\ell=1}^N h_{1,\ell}(x)\,b_{j,\ell}$, we deduce $h_{1,\ell}(x) = \sum_j b_{j,\ell}^{-1}(x+y_j)^{-1}$ and, similarly, $h_{2,\ell}(y) = \sum_i a_{i,\ell}^{-1}(x_i+y)^{-1}$. This gives

$$(x+y)^{-1} = \sum_{i,j,\ell} a_{i,\ell}^{-1} b_{j,\ell}^{-1}\,(x+y_j)^{-1}(x_i+y)^{-1}.$$

This expression must hold true on $(\mathbb{R}_+^*)^2$ and when $x,y\to 0^+$, the LHS goes to $+\infty$ while the RHS remains bounded. This is a contradiction. ■

5.3. Explicit formulae of a_r for scalar symbols ($u(x) = f(x)\,\mathbb{1}_N$)

When u is central, the operator defined by $I_{\alpha,k}(r_0,\dots,r_k)$ is equivalent to the operator defined by

$$\widetilde{I}_{\alpha,k}(r_0) := \lim_{r_j\to r_0} I_{\alpha,k}(r_0,\dots,r_k) = \tfrac{1}{k!}\,r_0^{-\alpha}.$$

Thus (4.4) reduces to

$$\begin{aligned}\tfrac{1}{(2\pi)^d}\int d\xi\,\xi_{\mu_1}\cdots\xi_{\mu_{2p}}\,f_k(\xi)[\,\mathbb{B}_k^{\mu_1\cdots\mu_{2p}}] &= g_d\,m[u^{-d/2-p}\otimes G(g)_{\mu_1\cdots\mu_{2p}}\,\mathbb{B}_k^{\mu_1\cdots\mu_{2p}}]\\ &= g_d\,G(g)_{\mu_1\cdots\mu_{2p}}\,u^{-d/2-p}\,m[\mathbb{B}_k^{\mu_1\cdots\mu_{2p}}]\end{aligned}$$

so the tedious part of the computation of a_r is to list all arguments $\mathbb{B}_k^{\mu_1\cdots\mu_{2p}}$ and to contract them with $G(g)_{\mu_1\cdots\mu_{2p}}$. This can be done with the help of a computer in any dimension for an arbitrary r. All formulae are obviously explicit. An eventual other step is to translate the results in terms of diffeomorphic and gauge invariants.

5.4. Application to quantum field theory

Second-order differential operators which are on-minimal have a great importance in physics and have justified their related heat-trace coefficients computation (to quote but a few see almost all references given here). For instance in the interesting work [18, 19], the operators P given in (1.1) are investigated under the restriction

$$u^{\mu\nu} = g^{\mu\nu}\,\mathbb{1} + \zeta\, X^{\mu\nu},$$

where ζ is a parameter (describing for $\zeta = 0$ the minimal theory), under the constraints for the normalized symbol $\widehat{X}(\sigma) := X^{\mu\nu}\sigma_\mu\sigma_\nu$ with $|\sigma|_g^2 = g^{\mu\nu}\sigma_\mu\sigma_\nu = 1$ given by

$$\widehat{X}(\sigma)^{\,2} = \widehat{X}(\sigma), \text{ for any } \sigma \in S^1_g\,, \tag{5.2}$$

$$\nabla_\rho\, X^{\mu\nu} = 0. \tag{5.3}$$

Here, ∇_ρ is a covariant derivative involving gauge and Christoffel connections. In covariant form, the operators are

$$P = -(g^{\mu\nu}\,\nabla_\mu\nabla_\nu + \zeta\, X^{\mu\nu}\,\nabla_\mu\nabla_\nu + Y).$$

Despite the restrictions (5.2)-(5.3) meaning that the operator $\widehat{X}$ is a projector and the tensor-endomorphism u is parallel, this covers the case of operators describing a quantized spin-1 vector fields like

$$P^\mu{}_\nu = -(\delta^\mu{}_\nu\,\nabla^2 + \zeta\,\nabla^\mu\nabla_\nu + Y^\mu{}_\nu),$$

or a Yang–Mills fields like

$$P^\mu{}_\nu = -(\delta^\mu{}_\nu\,D^2 - \zeta\,D^\mu D_\nu + R^\mu{}_\nu - 2F^\mu{}_\nu)$$

where $D_\mu := \nabla_\nu + A_\mu$ and A_μ, $F_{\mu\nu}$ are respectively the gauge and strength fields, or a perturbative gravity (see [18] for details).

Remark first that

$$\begin{aligned} H(x,\xi) &= u^{\mu\nu}\xi_\mu\xi_\nu = |\xi|_g^2\,[1 + \zeta\,\widehat{X}\,(\xi/|\xi|_g)], \text{ so that} \\ e^{-H(x,\xi)} &= [e^{-(1+\zeta)|\xi|_g^2} - e^{-|\xi|_g^2}]\,\widehat{X} + e^{-|\xi|_g^2}\,\mathbb{1}_V. \end{aligned}$$

Thus (1.10) becomes

$$\begin{aligned} a_0(x) &= \tfrac{1}{(2\pi)^d}\int d\xi\,[e^{-(1+\zeta)|\xi|_g^2} - e^{-|\xi|_g^2}]\ \mathrm{tr}\,\widehat{X} + \tfrac{1}{(2\pi)^d}\int e^{-|\xi|_g^2}\,\mathrm{tr}\ \mathbb{1}_V \\ &= [\int_{\sigma\in S^1_g} d\Omega(\sigma)\ \mathrm{tr}\,\widehat{X}(\sigma)]\,[\tfrac{1}{(2\pi)^d}\int_0^\infty dr\,r^{d-1}\,(e^{-(1+\zeta)r^2} - e^{-r^2})] + g_d\,N \\ &= \tfrac{\Gamma(d/2)}{2(2\pi)^d}\,[(1+\zeta)^{-d/2} - 1]\,[\int_{\sigma\in S^1_g} d\Omega(\sigma)\ \mathrm{tr}\,\widehat{X}(\sigma)] + g_d\,N. \end{aligned}$$

One has $g_d := \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} d\xi\, e^{-|\xi|^2_{g(x)}} = \frac{|g|^{1/2}}{2^d\,\pi^{d/2}}$ and

$$\int_{\sigma\in S^1_g} d\Omega(\sigma)\ \mathrm{tr}\,\widehat{X}(\sigma) = \mathrm{tr}(X^{\mu\nu})\int_{\sigma\in S^1_g} d\Omega(\sigma)\,\sigma_\mu\sigma_\nu\,.$$

Using (4.3), we can get

$$\int_{\sigma\in S^1_g} d\Omega(\sigma)\,\sigma_{\mu_1}\cdots\sigma_{\mu_{2p}} = \tfrac{2\,(2\pi)^d\,g_d}{\Gamma(d/2+p)}\,G(g)_{\mu_1\ldots\mu_{2p}},$$

so that we recover [18, (2.34)]:

$$a_0(x) = g_d\left[N + d^{-1}\,g_{\mu\nu}\,\mathrm{tr}(X^{\mu\nu})\Big((1+\zeta)^{-d/2}-1\Big)\right].$$

Now, let us consider the more general case

$$u^{\mu\nu} = g^{\mu\nu}u + \zeta\,X^{\mu\nu} \tag{5.4}$$

where u is a strictly positive matrix $u(x)\in M_N$ as in Section 4, $X^{\mu\nu}$ as before and assume $[u(x),X^{\mu\nu}(x)]=0$ for any $x\in(M,g)$ and μ,ν. Previous situation was $u=\mathbb{1}_V$, the unit matrix in M_N. Once Lemma 2.1 has been applied, the difficulty to compute $a_r(x)$ is to evaluate the operators $T_{k,p}$ defined by (2.15). Here we have $u[\sigma]=u+\zeta\,\widehat{X}(\sigma)$, where the two terms commute. With the notation

$$\widehat{X}_i := R_i[\widehat{X}(\sigma)],$$

we have

$$\begin{aligned}C_k(s,u[\sigma]) &= (1-s_1)R_0[u+\zeta\,\widehat{X}(\sigma)] + (s_1-s_2)R_1[u+\zeta\,\widehat{X}(\sigma)]+\ldots\\ &\qquad\cdots+(s_{k-1}-s_k)R_{k-1}[u+\zeta\,\widehat{X}(\sigma)] + s_kR_k[u+\zeta\,\widehat{X}(\sigma)]\\ &= C_k(s,u)+\zeta\Big[(1-s_1)\widehat{X}_0+(s_1-s_2)\widehat{X}_1+\cdots+(s_{k-1}-s_k)\widehat{X}_{k-1}+s_k\widehat{X}_k\Big]\end{aligned}$$

so that, using the fact that each $\widehat{X}_i$ is a projection with eigenvalues $\epsilon_i=0,1$:

$$\begin{aligned}e^{-r^2C_k(s,u[\sigma])} = e^{-r^2C_k(s,u)}\sum_{(\epsilon_i)\in\{0,1\}^{k+1}} & e^{-\zeta r^2[(1-s_1)\epsilon_0+(s_1-s_2)\epsilon_1+\cdots+(s_{k-1}-s_k)\epsilon_{k-1}+s_k\epsilon_k]}\times\\ &\times\widehat{X}_0^{\epsilon_0}(1-\widehat{X}_0)^{1-\epsilon_0}\cdots\widehat{X}_k^{\epsilon_k}(1-\widehat{X}_k)^{1-\epsilon_k}.\end{aligned}$$

Notice that $\widehat{X}_i^{\epsilon_i}(1-\widehat{X}_i)^{1-\epsilon_i} = [(1-\epsilon_i)g^{\mu\nu}+(2\epsilon_i-1)R_i(X^{\mu\nu})]\sigma_\mu\sigma_\nu$.
With the definition

$$I^{(\epsilon_i),\zeta}_{\alpha,k}(r_0,r_1,\ldots,r_k) := I_{\alpha,k}(r_0+\zeta\epsilon_0, r_1+\zeta\epsilon_1,\ldots,r_k+\zeta\epsilon_k),$$

the operators $T_{k,p}$ of (2.18) become

$$\begin{aligned}T_{k,p} =& \tfrac{\Gamma(d/2+p)}{2(2\pi)^d}\int_{S^{d-1}_g} d\Omega_g(\sigma)\,\sigma_{\mu_1}\cdots\sigma_{\mu_{2p}}\sigma_{\alpha_0}\sigma_{\beta_0}\cdots\sigma_{\alpha_k}\sigma_{\beta_k}\times\\ &\sum_{(\epsilon_i)\in\{0,1\}^{k+1}} I^{(\epsilon_i),\zeta}_{d/2+p,k}\Big(R_0(u),R_1(u),\ldots,R_k(u)\Big)\times\\ &\times[(1-\epsilon_0)g^{\alpha_0\beta_0}+(2\epsilon_0-1)R_0(X^{\alpha_0\beta_0})]\cdots[(1-\epsilon_k)g^{\alpha_k\beta_k}+(2\epsilon_k-1)R_k(X^{\alpha_k\beta_k})].\end{aligned} \tag{5.5}$$

The computations of these operators are attainable using the method given in Section 4, but with some more complicated combinatorial expressions requiring a computer. We will still get explicit formulae for $a_1(x)$ in any even dimension as in Theorem 4.5. The main combinatorial computation is to make the contractions between $G(g)_{\mu_1\ldots\mu_{2p}\alpha_0\beta_0\ldots\alpha_k\beta_k}$ from the first line of (5.5) with the operators of the last line applied on variables $\mathbb{B}_k^{\mu_1\ldots\mu_{2p}}$.
When $u=\mathbb{1}_V$ in (5.4), the operators in the second line of (5.5) are just the multiplication by the numbers $I_{d/2+p,k}(1+\zeta\epsilon_0,1+\zeta\epsilon_1,\ldots,1+\zeta\epsilon_k)$. Thus one gets explicit formulae for all coefficients $a_r(x)$ in any dimension.

6. Conclusion

On the search of heat-trace coefficients for Laplace type operators P with non-scalar symbol, we develop, using functional calculus, a method where we compute some operators $T_{k,p}$ acting on some (finite dimensional) Hilbert space and the arguments on which there are applied. This splitting allows to get general formulae for these operators and so, after a pure computational machinery will yield all coefficients a_r since there is no obstructions other than the length of calculations. The method is exemplified when the principal symbol of P has the form $g^{\mu\nu}u$ where u is a positive invertible matrix. It gives a_1 in any even dimension which is written both in terms of ingredients of P (analytic approach) or of diffeomorphic and gauge invariants (geometric approach). As just said, the method is yet ready for a computation of a_r with $r \geq 2$ for calculators patient enough, as well for the case $g^{\mu\nu}u + \zeta\, X^{\mu\nu}$ as in Section 5.4. Finally, the method answers a natural question about explicit expressions for all coefficients a_r: we proved that u-factorizability is always violated when the dimension is odd and it is preserved in even dimension d when $d/2 - r > 0$. We conjecture this always holds true in all even dimension.

A. Appendix

A.1. Some algebraic results

Let A be a unital associative algebra over $\mathbb{C}$, with unit $\mathbb{1}$.
Denote by $(C^*(A,A) = \oplus_{k\geq 0} C^k(A,A), \delta)$ the Hochschild complex where $C^k(A,A)$ is the space of linear maps $\omega : A^{\otimes^k} \to A$ and

$$(\delta\omega)[b_0 \otimes \cdots \otimes b_k] = b_0\omega[b_1 \otimes \cdots \otimes b_k] + \sum_{i=0}^{k} (-1)^i \omega[b_0 \otimes \cdots \otimes b_{i-1} \otimes b_{i+1} \otimes \cdots \otimes b_k] + (-1)^{k+1}\omega[b_0 \otimes \cdots \otimes b_{k-1}]b_k$$

for any $\omega \in C^k(A,A)$ and $b_0 \otimes \cdots \otimes b_k \in A^{\otimes^k}$.

Define the differential complex $(\mathfrak{T}^*A = \oplus_{k\geq 0} A^{\otimes^{k+1}}, d)$ with

$$d(a_0 \otimes \cdots \otimes a_k) = \mathbb{1} \otimes a_0 \otimes \cdots \otimes a_k + \sum_{i=0}^{k} (-1)^i a_0 \otimes \cdots \otimes a_{i-1} \otimes \mathbb{1} \otimes a_{i+1} \otimes \cdots \otimes a_k + (-1)^{k+1} a_0 \otimes \cdots \otimes a_k \otimes \mathbb{1}$$

for any $a_0 \otimes \cdots \otimes a_k \in A^{\otimes^{k+1}}$. Both $C^*(A,A)$ and $\mathfrak{T}^*A$ are graded differential algebras, the first one for the product

$$(\omega\,\omega')[b_1 \otimes \cdots \otimes b_{k+k'}] = \omega[b_1 \otimes \cdots \otimes b_k]\,\omega'[b_{k+1} \otimes \cdots \otimes b_{k+k'}]$$

and the second one for

$$(a_0 \otimes \cdots \otimes a_k)(a'_0 \otimes \cdots \otimes a'_{k'}) = a_0 \otimes \cdots \otimes a_k a'_0 \otimes \cdots \otimes a'_{k'} \in A^{\otimes^{k+k'+1}} = \mathfrak{T}^{k+k'}A.$$

The following result was proved in [25]:

Proposition A.1 *The map $\iota : \mathfrak{T}^* A \to C^*(A, A)$ defined by*

$$\iota(a_0 \otimes \cdots \otimes a_k)[b_1 \otimes \cdots \otimes b_k] := a_0 b_1 a_1 b_2 \cdots b_k a_k$$

is a morphism of graded differential algebras.

If A is central simple, then ι is injective, and if $A = M_N$ (algebra of $N \times N$ matrices) then ι is an isomorphism.

Recall that an associative algebra A is central simple if it is simple and its center is $\mathbb{C}$. Central simple algebras have the following properties, proved for instance in [26]:

Lemma A.2 *If B is a central simple algebra and C is a simple algebra, then $B \otimes C$ is a simple algebra. If moreover C is central simple, then $B \otimes C$ is also central simple.*

Proof (of Proposition A.1) A pure combinatorial argument shows that ι is a morphism of graded differential algebras for the structures given above.

Assume that A is central simple. The space $A^{\otimes^{k+1}}$ is an associative algebra for the product $(a_0 \otimes \cdots \otimes a_k) \cdot (a'_0 \otimes \cdots \otimes a'_k) = a_0 a'_0 \otimes \cdots \otimes a_k a'_k$, which is central simple by Lemma A.2. Let $J_k = \operatorname{Ker} \iota \cap A^{\otimes^{k+1}}$. Then, for any $\alpha = \sum_i a_{0,i} \otimes \cdots \otimes a_{k,i} \in J_k$, any $\beta = b_0 \otimes \cdots \otimes b_k \in A^{\otimes^{k+1}}$, and any $c_1 \otimes \cdots \otimes c_k \in A^{\otimes^k}$, one has

$$\iota(\alpha \cdot \beta)[c_1 \otimes \cdots \otimes c_k] = \sum_i a_{0,i} b_0 c_1 a_{1,i} b_1 c_2 \cdots b_{k-1} c_k a_{k,i} b_k = \iota(\alpha)[b_0 c_1 \otimes \cdots \otimes b_{k-1} c_k] b_k = 0,$$

so that $\alpha \cdot \beta \in J_k$. The same argument on the left shows that J_k is a two-sided ideal of the algebra $A^{\otimes^{k+1}}$, which is simple. Since ι is non zero ($\iota(\mathbb{1} \otimes \cdots \otimes \mathbb{1}) \neq 0$), one must have $J_k = 0$: this proves that ι is injective.

The algebra $A = M_N$ is central simple [26], so that ι is injective, and moreover the spaces $C^k(A, A)$ and $A^{\otimes^{k+1}}$ have the same dimensions: this shows that ι is an isomorphism. ■

Remark A.3 In [25], the graded differential algebras $C^*(A, A)$ and $\mathfrak{T}^* A$ are equipped with a natural Cartan operations of the Lie algebra A (where the bracket is the commutator) and it is shown that ι intertwines these Cartan operations. □

A.2. Some combinatorial results

Lemma A.4 *Given a family $a_0, \ldots, a_r$ of different complex numbers, we have*

$$i) \quad \sum_{n=0}^{r} a_n^s \prod_{m=0,\, m \neq n}^{r} (a_n - a_m)^{-1} = 0, \quad \text{for any } s \in \{0, 1, \ldots, r-1\}, \tag{A.1}$$

$$ii) \quad \prod_{m=0}^{r} (z - a_m)^{-1} = \sum_{n=0}^{r} (z - a_n)^{-1} \prod_{m=0,\, m \neq n}^{r} (a_n - a_m)^{-1}, \quad \forall z \in \mathbb{C} \backslash \{a_0, \ldots, a_r\}. \tag{A.2}$$

Proof i) If $\alpha(s) := \sum_{n=0}^{r} a_n^s \prod_{m=0,\, m \neq n}^{r} (a_n - a_m)^{-1}$ and

$$\beta(s) := \alpha(s) \prod_{0 \leq l < k \leq r} (a_k - a_l) = \sum_{n=0}^{r} (-1)^{r-n} a_n^s \prod_{\substack{0 \leq l < k \leq r \\ k \neq n,\, l \neq n}}^{r} (a_k - a_l)$$

then it is sufficient to show that $\beta(s) = 0$ for $s = 0, \dots, r-1$. Recall first that the determinant of a Vandermonde $p \times p$-matrix is

$$\det \begin{pmatrix} 1 & 1 & \cdots & 1 \\ b_1 & b_2 & \cdots & b_p \\ b_1^2 & b_2^2 & \cdots & b_p^2 \\ \vdots & \vdots & \cdots & \vdots \\ b_1^{p-1} & b_2^{p-1} & \cdots & b_p^{p-1} \end{pmatrix} = \prod_{1 \le j < i \le p} (b_i - b_j).$$

Thus

$$\det \begin{pmatrix} 1 & 1 & \cdots & 1 \\ a_0 & a_1 & \cdots & a_r \\ a_0^2 & a_1^2 & \cdots & a_r^2 \\ \vdots & \vdots & \cdots & \vdots \\ a_0^{r-1} & a_1^{r-1} & \cdots & a_r^{r-1} \\ a_0^s & a_1^s & \cdots & a_r^s \end{pmatrix} = \beta(s)$$

after an expansion of the determinant with respect to the last line. But this is zero since the last line coincides with the line $s+1$ of the matrix when $s = 0, \dots, r-1$.

ii) The irreducible fraction expansion of $f(z) = \frac{1}{(z-a_0)(z-a_1)\cdots(z-a_r)}$ is $\sum_{n=0}^{r} \frac{\mathrm{Res}(f)(a_n)}{z-a_n}$ yielding (A.2). ■

A.3. Few properties of functions $I_{d/2+k,k}$

We collect here some special combination of function $I_{d/2+k-r,k}$.

Let $g_1(r_0, r_1) := I_{d/2+1,2}(r_0, r_1, r_0)$. Then

$$\begin{aligned} \tfrac{1}{2}[g_1(r_0, r_1) + g_1(r_1, r_0)] &= \tfrac{1}{d}\,(r_0 r_1)^{-d/2}\ \tfrac{r_0^{d/2} - r_1^{d/2}}{r_0 - r_1} \\ &= \tfrac{1}{2m} \sum_{\ell=0}^{m-1} r_0^{-\ell-1}\, r_1^{\ell-m}, \quad \text{if } d = 2m. \end{aligned} \tag{A.3}$$

Let

$$\begin{aligned} g_2(r_0, r_1) := &- \tfrac{d}{2} I_{d/2+1,2}(r_0, r_1, r_0) \\ &+ \tfrac{d+2}{2}[r_1\, I_{d/2+2,3}(r_0, r_1, r_1, r_0) + r_1\, I_{d/2+2,3}(r_1, r_1, r_0, r_1) + r_0\, I_{d/2+2,3}(r_0, r_0, r_1, r_0)]. \end{aligned}$$

Then

$$\begin{aligned} g_2(r_0, r_1) &= \tfrac{1}{2d}\ \tfrac{(r_0 r_1)^{-d/2}\,(d\, r_0^{d/2+1} - d\, r_1 r_0^{d/2} - 4 r_1 r_0^{d/2} + d\, r_0 r_1^{d/2} - d\, r_1^{d/2+1} + 4 r_1^{d/2+1})}{(r_0 - r_1)^2} \\ &= \tfrac{1}{2m} \sum_{\ell=0}^{m-1} (m - 2\ell)\, r_0^{-\ell-1}\, r_1^{\ell-m}, \qquad \text{if } d = 2m. \end{aligned} \tag{A.4}$$

Let

$$\begin{aligned} g_3(r_0, r_1) := &\tfrac{(d+2)^2}{2}\, r_0\, I_{d/2+2,3}(r_0, r_0, r_1, r_0) \\ &+ (d+2)(d+4)[-{r_0}^2\, I_{d/2+3,4}(r_0, r_0, r_0, r_1, r_0) - \tfrac{1}{2} r_0\, r_1\, I_{d/2+3,4}(r_0, r_0, r_1, r_1, r_0)]. \end{aligned} \tag{A.5}$$

Then,

$$\begin{aligned}
&\tfrac{1}{2}[g_3(r_0,r_1)+g_3(r_1,r_0)]\\
&\quad=\tfrac{1}{12d}\,\frac{(r_0r_1)^{-d/2}\Big[d^2(r_0-r_1)^2\Big(r_0^{d/2}-r_1^{d/2}\Big)-2d(r_0-r_1)\Big(r_1r_0^{d/2}+2r_0^{d/2+1}+r_0r_1^{d/2}+2r_1^{d/2+1}\Big)+24r_0r_1\Big(r_0^{d/2}-r_1^{d/2}\Big)\Big]}{(r_0-r_1)^3}\\
&\quad=\tfrac{1}{6m}\sum_{\ell=0}^{m-1}(m^2-2m-3\ell(m-1-\ell))\,r_0^{-\ell-1}\,r_1^{\ell-m},\qquad \text{if } d=2m.
\end{aligned}\tag{A.6}$$

A.4. Diffeomorphism invariance and gauge covariance of P

The operator P in (1.1) is given in terms of $u^{\mu\nu}, v^\mu, w$, which are not well adapted to study the changes of coordinates and gauge transformations.

Given a change of coordinates (c.c.) $x \xrightarrow{\text{c.c.}} x'$, let $J^\nu_\mu := \partial_\mu x'^\mu$ and $|J| := \det(J^\nu_\mu)$, so that

$$\partial_\mu \xrightarrow{\text{c.c.}} J^{-1}{}^\alpha_\mu\partial_\alpha,\qquad g_{\mu\nu}\xrightarrow{\text{c.c.}} J^{-1}{}^\rho_\mu J^{-1}{}^\sigma_\nu g_{\rho\sigma},\qquad g^{\mu\nu}\xrightarrow{\text{c.c.}} J^\mu_\rho J^\nu_\sigma g^{\rho\sigma},\qquad |g|\xrightarrow{\text{c.c.}}|J|^{-2}|g|$$

where $|g|=\det(g_{\mu\nu})$. Denote by γ a gauge transformation, local in the trivialization of V in which P is written (*i.e.* γ is a map from the open subset of M which trivializes V to the gauge group $GL_N(\mathbb{C})$). A section s of V performs the transformations $s\xrightarrow{\text{c.c.}}s$ (diffeomorphism-invariant) and $s\xrightarrow{\text{g.t.}}\gamma s$ (where "g.t." stands for gauge transformation).
The proof of the following lemma is a straightforward computation:

Lemma A.5 *The differential operator P is well defined on sections of V if and only if $u^{\mu\nu}$, v^μ and w have the following transformations:*

$$u^{\mu\nu}\xrightarrow{c.c.}J^\mu_\rho J^\nu_\sigma u^{\rho\sigma},\qquad u^{\mu\nu}\xrightarrow{g.t.}\gamma u^{\mu\nu}\gamma^{-1},\tag{A.7}$$

$$v^\mu\xrightarrow{c.c.}J^\mu_\rho v^\rho+(\partial_\sigma J^\mu_\rho)u^{\rho\sigma},\qquad v^\mu\xrightarrow{g.t.}\gamma v^\mu\gamma^{-1}+2\gamma u^{\mu\nu}(\partial_\nu\gamma^{-1}),\tag{A.8}$$

$$w\xrightarrow{c.c.}w,\qquad w\xrightarrow{g.t.}\gamma w\gamma^{-1}+\gamma v^\mu(\partial_\mu\gamma^{-1})+\gamma u^{\mu\nu}(\partial_\mu\partial_\nu\gamma^{-1}).\tag{A.9}$$

As these relations show, neither v^μ nor w have simple transformations under changes of coordinates or gauge transformations.

It is possible to parametrize P using structures adapted to changes of coordinates and gauge transformations. Let us fix a (gauge) connection A_μ on V and denote by $\nabla_\mu := \partial_\mu + A_\mu$ its associated covariant derivative on sections of V. For any section s of V, one then has:

$$A_\mu\xrightarrow{\text{c.c.}}J^{-1}{}^\alpha_\mu A_\alpha,\quad A_\mu\xrightarrow{\text{g.t.}}\gamma A_\mu\gamma^{-1}+\gamma(\partial_\mu\gamma^{-1}),\quad \nabla_\mu s\xrightarrow{\text{c.c.}}J^{-1}{}^\alpha_\mu\nabla_\alpha s,\quad \nabla_\mu s\xrightarrow{\text{g.t.}}\gamma\nabla_\mu s.\tag{A.10}$$

Lemma A.6 *The differential operator*

$$s\mapsto Qs := -(|g|^{-1/2}\nabla_\mu|g|^{1/2}u^{\mu\nu}\nabla_\nu+p^\mu\nabla_\mu+q)\,s\tag{A.11}$$

is well defined on sections of V if and only if $u^{\mu\nu}$, p^μ and q have the following transformations:

$$u^{\mu\nu}\xrightarrow{c.c.}J^\mu_\rho J^\nu_\sigma u^{\rho\sigma},\qquad p^\mu\xrightarrow{c.c.}J^\mu_\rho p^\rho,\qquad q\xrightarrow{c.c.}q,\tag{A.12}$$

$$u^{\mu\nu}\xrightarrow{g.t.}\gamma u^{\mu\nu}\gamma^{-1},\qquad p^\mu\xrightarrow{g.t.}\gamma p^\mu\gamma^{-1},\qquad q\xrightarrow{g.t.}\gamma q\gamma^{-1}.\tag{A.13}$$

It is equal to P when (the $u^{\mu\nu}$ are the same in P and Q)

$$v^\mu=\tfrac{1}{2}(\partial_\nu\log|g|)u^{\mu\nu}+\partial_\nu u^{\mu\nu}+u^{\mu\nu}A_\nu+A_\nu u^{\mu\nu}+p^\mu,\tag{A.14}$$

$$w=\tfrac{1}{2}(\partial_\mu\log|g|)u^{\mu\nu}A_\nu+(\partial_\mu u^{\mu\nu})A_\nu+u^{\mu\nu}(\partial_\mu A_\nu)+A_\mu u^{\mu\nu}A_\nu+p^\mu A_\mu+q.\tag{A.15}$$

Proof Combining (A.10), (A.12) and (A.13), the operator $s \mapsto -(p^\mu \nabla_\mu + q)s$ is well behaved under changes of coordinates and gauge transformations. Let $X := |g|^{-1/2}\nabla_\mu |g|^{1/2} u^{\mu\nu}\nabla_\nu$ (a matrix valued "Laplace–Beltrami operator"). Then, using (A.10) and (A.12), one gets

$$\begin{aligned}
X &\xrightarrow{\text{c.c.}} |J||g|^{-1/2} J^{-1}{}^{\alpha}_{\mu} \nabla_\alpha |J|^{-1} |g|^{1/2} J^\mu_\rho J^\nu_\sigma u^{\rho\sigma} J^{-1}{}^{\beta}_{\nu} \nabla_\beta \\
&= |J||g|^{-1/2} J^{-1}{}^{\alpha}_{\mu} \partial_\alpha |J|^{-1} |g|^{1/2} J^\mu_\rho u^{\rho\sigma}\nabla_\sigma + J^{-1}{}^{\alpha}_{\mu} J^\mu_\rho A_\alpha u^{\rho\sigma}\nabla_\sigma \\
&= |J| J^{-1}{}^{\alpha}_{\mu} J^\mu_\rho (\partial_\alpha |J|^{-1}) u^{\rho\sigma}\nabla_\sigma + |g|^{-1/2} J^{-1}{}^{\alpha}_{\mu} J^\mu_\rho (\partial_\alpha |g|^{1/2}) u^{\rho\sigma}\nabla_\sigma \\
&\quad + J^{-1}{}^{\alpha}_{\mu} (\partial_\alpha J^\mu_\rho) u^{\rho\sigma}\nabla_\sigma + J^{-1}{}^{\alpha}_{\mu} J^\mu_\rho \partial_\alpha u^{\rho\sigma}\nabla_\sigma + A_\rho u^{\rho\sigma}\nabla_\sigma \\
&= \nabla_\rho u^{\rho\sigma}\nabla_\sigma + |g|^{-1/2}(\partial_\rho |g|^{1/2}) u^{\rho\sigma}\nabla_\sigma \\
&\quad + |J|(\partial_\rho |J|^{-1}) u^{\rho\sigma}\nabla_\sigma + J^{-1}{}^{\alpha}_{\mu}(\partial_\alpha J^\mu_\rho) u^{\rho\sigma}\nabla_\sigma
\end{aligned}$$

which is equal to X since $|J|\partial_\rho |J|^{-1} = -|J|^{-1}\partial_\rho |J| = -\partial_\rho \log|J| = -J^{-1}{}^{\alpha}_{\mu}(\partial_\rho J^\mu_\alpha)$ (Jacobi's formula) and $\partial_\alpha J^\mu_\rho = \partial_\alpha \partial_\rho x'^\mu = \partial_\rho \partial_\alpha x'^\mu = \partial_\rho J^\mu_\alpha$. Similarly, using (A.10) and (A.13), one obtains

$$|g|^{1/2} u^{\mu\nu}\nabla_\nu s \xrightarrow{\text{g.t.}} \gamma |g|^{1/2} u^{\mu\nu}\nabla_\nu s \quad \text{(it behaves like a section of } V\text{)},$$

so that $Xs \xrightarrow{\text{g.t.}} \gamma X s$. This proves that $Q = -X - (p^\mu \nabla_\mu + q)$ is well defined.

The expansion of X gives

$$\begin{aligned}
X &= |g|^{-1/2}\partial_\mu |g|^{1/2} u^{\mu\nu}(\partial_\nu + A_\nu) + A_\nu u^{\mu\nu}(\partial_\nu + A_\nu) \\
&= |g|^{-1/2}(\partial_\mu |g|^{1/2}) u^{\mu\nu}\partial_\nu + |g|^{-1/2}(\partial_\mu |g|^{1/2}) u^{\mu\nu} A_\nu + (\partial_\mu u^{\mu\nu})\partial_\nu + (\partial_\mu u^{\mu\nu}) A_\nu \\
&\quad + u^{\mu\nu}\partial_\mu \partial_\nu + u^{\mu\nu}(\partial_\mu A_\nu) + u^{\mu\nu} A_\nu \partial_\mu + A_\mu u^{\mu\nu}\partial_\nu + A_\mu u^{\mu\nu} A_\nu \\
&= u^{\mu\nu}\partial_\mu \partial_\nu + \tfrac{1}{2}(\partial_\mu \log|g|) u^{\mu\nu}\partial_\nu + (\partial_\mu u^{\mu\nu})\partial_\nu + u^{\mu\nu} A_\nu \partial_\mu + A_\mu u^{\mu\nu}\partial_\nu \\
&\quad + \tfrac{1}{2}(\partial_\mu \log|g|) u^{\mu\nu} A_\nu + (\partial_\mu u^{\mu\nu}) A_\nu + u^{\mu\nu}(\partial_\mu A_\nu) + A_\mu u^{\mu\nu} A_\nu
\end{aligned}$$

which, combined with the contributions of $-(p^\mu \nabla_\mu + q)$, gives (A.14) and (A.15). ■

Contrary to the situation in [1, Section 1.2.1], one cannot take directly $p = 0$ in (A.11) since we cannot always solve A_μ in (A.14) to write it in terms of $u^{\mu\nu}$, v^μ, w.

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