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Covariant derivative expansion of the heat kernel

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Abstract. Using the technique of labeled operators, compact explicit expressions are given for all traced heat kernel coefficients containing zero, two, four and six covariant derivatives, and for diagonal coefficients with zero, two and four derivatives. The results apply to boundaryless flat space-times and arbitrary non-Abelian scalar and gauge background fields.

1 Introduction and conclusions

Ever since its introduction by Schwinger [1], the heat kernel of Laplace-type operators has been a useful tool to deal with one loop effective actions in quantum field theory. This due to the fact that the heat kernel provides a manifestly gauge invariant regularization of ultraviolet divergences. An additional virtue, is that, unlike the effective action, the heat kernel is a one-valued functional. The heat kernel can be applied to study spectral densities of Klein–Gordon operators and in the proof of index theorems [2,3], to compute the ζ-function [4] and the anomalies of Dirac operators [5], to deal with chiral gauge theories [6] and models of QCD [7], to the Casimir effect [8], to compute black hole entropies [9], etc. Exact calculations of the heat kernel at coincident points are available in particular manifolds [10, 11] or for configurations subjected to suitable algebraic constraints (of the constant curvature type) [12–14]. In the general case an asymptotic expansion in powers of the proper time, the Seeley–DeWitt expansion [15,16], is available. The coefficients of the expansion have been computed to rather high orders in several setups, including curved spaces with and without boundary, and in presence of non-Abelian gauge fields and non-Abelian scalar fields, using different methods [6, 17–24]. The heat kernel expansion at finite temperature has been discussed in [25,26]. A generalized heat kernel expansion around non-c-number mass terms has been introduced in [27–29]. The extension to non-commutative quantum field theory has been presented in [30].

The standard heat kernel expansion can be regarded as a double expansion in the strength and in the number of derivatives of the background fields. It is therefore most suitable for external fields which are both weak and adiabatic, i.e., of slow space-time variation. A resummation of this expansion is provided by covariant perturbation theory [31]. Perturbation theory assumes weak but not necessarily adiabatic fields. In this paper we study a different resummation, namely, a covariant derivative expansion [32–34]. The terms of this expansion have a given number of covariant derivatives but any number of scalar fields (these fields playing the role a non-Abelian local mass term). So the fields are assumed to be adiabatic (and the gauge fields weak, to preserve gauge invariance) but the scalar fields may be strong. Using the technique of labeled operators, we are able to write in finite form the contributions to the traced heat kernel classified by the number of derivatives. Such contributions can also be regarded as generating functions for all the heat kernel coefficients of the standard Seeley–DeWitt expansion with a fixed number of derivatives. Explicit results are presented for zero, two, four and six derivatives, involving 1, 1, 6 and 52 summands, respectively. These results hold for boundaryless flat space-time but non-Abelian gauge and scalar fields. Extension to curved space-time should also be possible using the symbols method. A covariant derivative expansion to four derivatives has been obtained in [35] for the diagonal heat kernel and in [36] for the effective action, for curved space-time in the case of minimal (i.e. Abelian) scalar field and no gauge connection.

In Sect. 2 we define the covariant derivative expansion for the trace of the heat kernel and work out the lower order terms. Although the calculation could be done from scratch using the method of symbols, a shorter path is provided by the method of Chan [32] which was devised for the effective action. In that section results are presented to four derivatives. We show that after expansion of our results in powers of the scalar field the standard coefficients are recovered. Section 3 is devoted to explaining the technique of labeled operators [33,34,37,38]. Such a procedure allows one to develop a calculus to deal with functions of non-commuting variables. The non-commutative version of the ordinary derivative is shown to satisfy the Leibniz and chain rules, as well as to yield a non-commutative version of the Taylor expansion. In Sect. 4 the diagonal heat kernel coefficients, within the derivative expansion, are ob-

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tained to four derivatives. This is done through functional variation of the traced coefficients. Unlike the standard expansion, in the resummed expansion one finds that each diagonal term comes from the traced term of the same order. This yields a consistency condition that is verified by our formulas. Section 5 gives the six derivative contribution. It is based on previous results for the effective action found in [39]. Here one important issue is that of finding either a short or a systematic expression for the result. This is due to the existence of identities among the possible gauge invariant structures, coming from integration by parts and Jacobi identities. In that section we give a relatively short expression for the six derivative contribution, which contains 52 different gauge invariant structures. In Sect. 6 we study the problem of finding a standard basis of structures for the derivative expansion of generic gauge invariant functionals. The corresponding problem in the context of the standard heat kernel expansion has been treated before by Müller [40, 41]. Some subtleties appear for the derivative expansion because the analogous of the Seeley–DeWitt coefficients are now functions (of labeled operators). So, for instance, even if the elements of a basis are complete and linearly independent it does not directly follow that the coefficients must be unique; it is at least necessary to impose permutation symmetry restrictions to the functions which play the role of coefficients of the expansion. In this last section we construct standard basis of gauge invariant structures for functionals with zero, two, four and six derivatives, with 1, 1, 6 and 37 elements, respectively. It is worth noticing that, similarly to what happens for the standard heat kernel expansion [30], all the results presented here apply directly to non-commutative quantum field theory. This is particularly clear when such theories are formulated within the quantum phase space approach [42], which only requires to replace the integral over coordinates by a trace on X-space. Indeed, at no place do we use special commutation properties for our symbols, except $[\partial_\mu, \partial_\nu] = 0$ which holds in the non-commutative case too.

2 Covariant derivative expansion of the heat kernel

Our goal is to obtain a derivative expansion for the heat kernel of the Klein–Gordon operator

$$K = D_\mu^2 + X\,. \tag{2.1}$$

Here $X(x)$ is a multiplicative operator (i.e. an ordinary function) which is a matrix in some internal space, $D_\mu = \partial_\mu + V_\mu(x)$ is the covariant derivative, $V_\mu(x)$ being a matrix in internal space. Space-time is Euclidean and flat, without boundaries and has dimension d. K acts on matter fields in the fundamental representation.

The standard heat kernel expansion is of the form

$$\langle x|\mathrm{e}^{\tau K}|x\rangle = \frac{1}{(4\pi\tau)^{d/2}} \sum_{n=0}^{\infty} \tau^n\, a_n(x)\,. \tag{2.2}$$

This is an asymptotic expansion where the a_n, known as (diagonal) Seeley–DeWitt coefficients, are τ-independent local gauge covariant polynomials of dimension $2n$. They are constructed with X and D_μ in gauge covariant combinations. One can choose to order the expansion by powers of τ or, equivalently, by the mass dimension carried by the external fields V_μ and X and their derivatives. The quantities ∂_μ, V_μ and X have dimension 1,1,2 respectively. In spaces with boundary, n may take half-integer values [43], but in our case the index n is a non-negative integer. The lowest order terms are

$$\begin{aligned} a_0 &= 1\,, \\ a_1 &= X\,, \\ a_2 &= \frac{1}{2}X^2 + \frac{1}{6}X_{\mu\mu} + \frac{1}{12}Z_{\mu\nu}^2\,. \end{aligned} \tag{2.3}$$

In the derivative expansion the terms are classified by the number of covariant derivatives they carry, rather than the mass dimension they carry (as in the standard heat kernel expansion) so

$$\langle x|\mathrm{e}^{\tau K}|x\rangle = \frac{1}{(4\pi\tau)^{d/2}} \sum_{n=0}^{\infty} \tau^n A_n(x)\,, \tag{2.4}$$

where $A_n(x)$ depends on τ and contains $2n$ covariant derivatives. In this counting, X counts as zeroth order, $[D_\mu, X]$ as first order, $Z_{\mu\nu} = [D_\mu, D_\nu]$ as second order, and so on. (Counting the dimension carried by the background fields and by τ, A_n has dimension $2n$.) Technically, the covariant derivative expansion can be defined by introducing a bookkeeping parameter λ by means of $X(x) \to X(\lambda x)$ and $V_\mu(x) \to \lambda V_\mu(\lambda x)$, and then expanding the functional $\langle \lambda^{-1}x|\mathrm{e}^{\tau K(\lambda)}|\lambda^{-1}x\rangle$ in powers of λ. The derivative expansion is a resummation of the standard expansion, namely, if a_n^q denotes the pieces of a_n with exactly $2q$ covariant derivatives (and so with $n-q$ X's)

$$A_q(x) = \sum_{n\geq q} \tau^{n-q} a_n^q(x)\,. \tag{2.5}$$

In what follows we will set $\tau = 1$, i.e. remove τ from the formulas, since it can be restated at any moment by standard dimensional counting. Thus, for instance

$$\langle x|\mathrm{e}^{K}|x\rangle = \frac{1}{(4\pi)^{d/2}} \sum_{n=0}^{\infty} A_n(x)\,. \tag{2.6}$$

In each A_n, X appears to all orders. The prescription to restore τ is simply to make the replacement $X \to \tau X$, plus $A_n \to \tau^n A_n$.

For many purposes it is often sufficient to work with the functional trace of the heat kernel,

$$\mathrm{Tr}\,\mathrm{e}^{K} = \int \mathrm{d}^d x\ \mathrm{tr}\langle x|\mathrm{e}^{K}|x\rangle\,. \tag{2.7}$$

The symbol Tr refers to the full trace on space-time and internal spaces. We will use tr to denote the trace in the

internal space only. Introducing the short-hand notation[1]

$$\langle\ \rangle := \frac{1}{(4\pi\tau)^{d/2}} \int \mathrm{d}^d x\ \mathrm{tr}(\ )\ , \tag{2.8}$$

the standard and derivative expansions take the form

$$\mathrm{Tr}\,\mathrm{e}^K = \sum_{n=0}^{\infty} \langle a_n(x)\rangle = \sum_{n=0}^{\infty} \langle A_n(x)\rangle\ . \tag{2.9}$$

In $\mathrm{Tr}\,\mathrm{e}^K$ one can use simpler coefficients, b_n and B_n, which coincide with a_n and A_n, respectively, modulo by parts integration and the trace cyclic property, so that

$$\langle b_n\rangle = \langle a_n\rangle\ , \quad \langle B_n\rangle = \langle A_n\rangle\ . \tag{2.10}$$

In particular,

$$\mathrm{Tr}\,\mathrm{e}^K = \sum_{n=0}^{\infty} \langle B_n\rangle\ . \tag{2.11}$$

Whereas the coefficients A_n and the functionals $\langle B_n\rangle$ are uniquely defined, there is an ambiguity in the choice of B_n which is exploited to choose them as simple as possible. The coefficients A_n can be obtained from the B_n (see Sect. 4).

The calculation of the coefficients B_n can be done using the method of symbols [44,45] (actually, this methods provides A_n from which B_n is obtained). In addition to the derivation of the coefficients an important part of the calculation is to find a simple expression for them, that is, removing redundancies coming from the trace cyclic property, integration by parts and Bianchi identities. Because much work has been devoted to the covariant derivative expansion of the effective action, we have found it practical to start from that functional where much of the simplification work has already been done. The most useful results for our purposes are found in the work of Chan [32] who obtains the derivative expansion of the effective action with a minimum of terms up to four derivatives. This work was later extended to six derivatives in [39]. There we find (making explicit terms up to second order)

$$\mathrm{Tr}\log K = \int \frac{\mathrm{d}^d x \mathrm{d}^d k}{(2\pi)^d}\ \mathrm{tr}\left(-\log N + \frac{k^2}{d} N_\mu^2 + \dots\right)\ , \tag{2.12}$$

where

$$N = (k^2 - X)^{-1}\ , \quad N_\mu = [D_\mu, N]\,. \tag{2.13}$$

In what follows we will consistently use the convention[2] $Y_{\mu I} = [D_\mu, Y_I]$ where Y_I is an object (such as N, X or Z) with an ordered set of Lorentz indices I. So for instance[3]

$$X_{\mu\nu} = [D_\mu, [D_\nu, X]]\,,$$

$$Z_{\mu\nu\lambda} = [D_\mu, Z_{\nu\lambda}] = [D_\mu, [D_\nu, D_\lambda]]\,. \tag{2.14}$$

The formula (2.12) holds modulo a counterterm action which must be a local polynomial (in X, V_μ and ∂_μ) of degree at most d. Such counterterms depend on the renormalization prescription chosen. The derivative expansion of the effective action can be written as

$$\mathrm{Tr}\log K = \int \frac{\mathrm{d}^d x \mathrm{d}^d k}{(2\pi)^d} \sum_{n=0}^{\infty} k^{2n} \frac{\Gamma(d/2)}{\Gamma(n+d/2)}\ \mathrm{tr}\,(F_n)\ . \tag{2.15}$$

Each F_n is gauge covariant, contains a number $2n$ of D_μ's and a number $2n$ of N's, and has no explicit dependence on the space-time dimension d. To four derivatives

$$\begin{aligned} F_0 &= -\log N\,, \\ F_1 &= \frac{1}{2} N_\mu^2\,, \\ F_2 &= N_\mu^2 N_\nu^2 - \frac{1}{2}(N_\mu N_\nu)^2 - (N N_{\mu\mu})^2 - 2 N Z_{\mu\nu} N N_\mu N_\nu \\ &\quad - \frac{1}{2}(Z_{\mu\nu} N^2)^2\,. \end{aligned} \tag{2.16}$$

These terms were obtained in [32][4]. The six derivative term F_3 is given in (5.1). It was obtained in [39] and contains 45 terms. In this section we concentrate on terms up to four derivatives and defer the treatment of the six derivative terms to Sect. 5. We will not consider terms with eight or more derivatives in this work.

First of all we will translate the expansion (2.15) to an expansion for the heat kernel:

$$\begin{aligned} \mathrm{e}^K &= \int_\Gamma \frac{\mathrm{d}z}{2\pi\mathrm{i}} \frac{\mathrm{e}^z}{z-K} = \int_\Gamma \frac{\mathrm{d}z}{2\pi\mathrm{i}} \mathrm{e}^z \frac{\mathrm{d}}{\mathrm{d}z} \log(K-z) \\ &= -\int_\Gamma \frac{\mathrm{d}z}{2\pi\mathrm{i}} \mathrm{e}^z \log(K-z)\,. \end{aligned} \tag{2.17}$$

Here Γ is a positively oriented path in the z complex plane enclosing the eigenvalues of K. Because the large eigenvalues of K lie on the real negative axis, the path is taken starting and ending at $-\infty$. Next we apply Chan's formula (2.15) to $\mathrm{Tr}\log(K-z)$, i.e., with the replacement $X \to X - z$. The first thing to note is that the counterterm ambiguities do not survive in the heat kernel, since a polynomial in z does not give a contribution to the integral in (2.17). Taking Tr in (2.17) and inserting (2.15), one finds that all non-explicit dependence on k_μ comes in the form $X - k^2 - z$. Making the shift $z \to z - k^2$ removes all dependence on k_μ in F_n. (Such change of variables is justified at the level of asymptotic expansions we are considering.) Straightforward momentum integration gives then

$$\mathrm{Tr}\,\mathrm{e}^K = -\sum_{n=0}^{\infty} \int_\Gamma \frac{\mathrm{d}z}{2\pi\mathrm{i}} \mathrm{e}^z \langle F_n\rangle\ ; \tag{2.18}$$

[1] Our notational conventions are summarized in Appendix A.

[2] Here and elsewhere in this work Y stands for a generic matrix-valued function.

[3] Note that in [39] the convention $Y_{I\mu} = [D_\mu, Y_I]$ is used instead. Also $F_{\mu\nu}$ there corresponds to $\mathrm{i}Z_{\mu\nu}$ here.

[4] Note that the sign of the fourth term of F_2 is incorrect in [32].

that is,

$$B_n = -\int_\Gamma \frac{\mathrm{d}z}{2\pi\mathrm{i}} \mathrm{e}^z F_n \tag{2.19}$$

(perhaps modulo integration by parts and cyclic property). In this formula the quantities F_n are given by the same expressions (2.16) where now

$$N = (z - X)^{-1} . \tag{2.20}$$

The integration over z is easily done for the zeroth order term (undoing the steps in (2.17))

$$B_0 = \int_\Gamma \frac{\mathrm{d}z}{2\pi\mathrm{i}} \mathrm{e}^z \log N = \int_\Gamma \frac{\mathrm{d}z}{2\pi\mathrm{i}} \frac{\mathrm{e}^z}{z - X} = \mathrm{e}^X . \tag{2.21}$$

For B_1, we first expand the covariant derivative using the identity

$$N_\mu = N X_\mu \, N, \tag{2.22}$$

so that z appears only in N outside covariant derivatives

$$F_1 = \frac{1}{2} N^2 X_\mu N^2 X_\mu \tag{2.23}$$

(exploiting the cyclic property to move the last N to the first place).

When this F_1 is inserted in (2.19) the integral over z cannot be readily done because z appears in two places and the operators do not commute in general. Here we apply the technique of labeling the operators [33,34,37,38]: relative to the two X_μ in (2.23) there are three positions, namely, the position 1 at the left of the first (leftmost) X_μ, the position 2, in between the two X_μ and the position 3, after the second X_μ. (Operators at position 3 can be moved to position 1 by the cyclic property.) The operators relative to which the positions are defined (the two X_μ in this case) are named "fixed operators". The other operators are then labeled according to their position relative to the fixed operators and moved to the left (or to any convenient location in the expression). In this way we can rewrite (2.23) as

$$F_1 = \frac{1}{2} N_1^2 N_2^2 X_\mu X_\mu = \frac{1}{2} \frac{1}{(z - X_1)^2} \frac{1}{(z - X_2)^2} X_\mu^2 . \tag{2.24}$$

The labels 1 and 2 indicate at which position the labeled operators N_1 and N_2 (or X_1, X_2) should be inserted (relative to the fixed operators $X_\mu X_\mu$). The point of following this procedure is that the labeled operators are effectively c-numbers: similar to the time-ordered product or the normal product, they can be written in any order since their true position is given by their label. Because they are c-numbers, nothing prevents us from doing the z integration as for ordinary functions. We refer to Sect. 3 for details on the use and properties of labeled operators. Their use is crucial for the rest of the paper. After integration over z we obtain

$$\langle B_1 \rangle = \big\langle f(X_1, X_2) X_\mu^2 \big\rangle \tag{2.25}$$

where X_1 is X located at position 1 and X_2 is X at position 2. $f(X_1, X_2)$ is the ordinary function $f(x, y)$ evaluated at X_1 and X_2, with

$$f(x, y) = -\frac{1}{2} \int_\Gamma \frac{\mathrm{d}z}{2\pi\mathrm{i}} \mathrm{e}^z \frac{1}{(z - x)^2} \frac{1}{(z - y)^2}$$
$$= \frac{\mathrm{e}^x - \mathrm{e}^y}{(x - y)^3} - \frac{1}{2} \frac{\mathrm{e}^x + e^y}{(x - y)^2} . \tag{2.26}$$

(By definition Γ always encloses the poles, in this case at x and y.)

The right-hand side of (2.25) can be regarded as the generating function for all the Seeley–DeWitt coefficients with two covariant derivatives. Indeed, making a series expansion in X one obtains (using the cyclic property in the second equality)

$$\begin{aligned}\langle B_1 \rangle &= \Big\langle \Big(-\frac{1}{12} - \frac{1}{24}(X_1 + X_2) - \frac{1}{80}(X_1^2 + X_2^2) \\ &\qquad - \frac{1}{60} X_1 X_2 + \dots \Big) X_\mu^2 \Big\rangle \\ &= \Big\langle -\frac{1}{12} X_\mu^2 - \frac{1}{12} X X_\mu^2 - \frac{1}{40} X^2 X_\mu^2 \\ &\qquad - \frac{1}{60} X X_\mu X X_\mu + \dots \Big\rangle .\end{aligned} \tag{2.27}$$

To the order shown, this reproduces the pieces with two covariant derivatives in b_3, b_4 and b_5 [17].

For the four derivative term we proceed similarly. Expanding the covariant derivatives of N one finds

$$\begin{aligned}F_2 &= (N^2 X_\mu N^2 X_\mu)^2 - \frac{1}{2}(N^2 X_\mu N^2 X_\nu)^2 \\ &\quad -4(N^3 X_\mu N X_\mu)^2 - (N^3 X_{\mu\mu})^2 \\ &\quad -4N^3 X_\mu N X_\mu N^3 X_{\nu\nu} - 2N^2 X_\mu N^2 X_\nu N^2 Z_{\mu\nu} \\ &\quad -\frac{1}{2}(N^2 Z_{\mu\nu})^2 \\ &= N_1^2 N_2^2 N_3^2 N_4^2 (X_\mu^2)^2 - \frac{1}{2} N_1^2 N_2^2 N_3^2 N_4^2 (X_\mu X_\nu)^2 \\ &\quad -4N_1^3 N_2 N_3^3 N_4 (X_\mu^2)^2 - N_1^3 N_2^3 X_{\mu\mu}^2 \\ &\quad -4N_1^3 N_2 N_3^3 X_\mu^2 X_{\nu\nu} - 2N_1^2 N_2^2 N_3^2 X_\mu X_\nu Z_{\mu\nu} \\ &\quad -\frac{1}{2} N_1^2 N_2^2 Z_{\mu\nu}^2 .\end{aligned} \tag{2.28}$$

The integrals over z involved in the computation of the B_n are of the form

$$I_{r_1, r_2, \dots, r_n}(X_1, X_2, \dots, X_n) := \int_\Gamma \frac{\mathrm{d}z}{2\pi\mathrm{i}} \mathrm{e}^z N_1^{r_1} N_2^{r_2} \dots N_n^{r_n} . \tag{2.29}$$

They can be computed from the basic integrals

$$\begin{aligned}&I_n^0(X_1, X_2, \dots, X_n) \\ &:= \int_\Gamma \frac{\mathrm{d}z}{2\pi\mathrm{i}} \mathrm{e}^z N_1 N_2 \dots N_n = \sum_{i=1}^n \mathrm{e}^{X_i} \prod_{j \neq i} \frac{1}{X_i - X_j}\end{aligned} \tag{2.30}$$

using

$$I_{r_1, r_2, \dots, r_n}(X_1, X_2, \dots, X_n) \tag{2.31}$$

$$= \prod_{i=1}^{n} \frac{1}{(r_i-1)!} \left(\frac{\partial}{\partial X_i}\right)^{r_i-1} I_n^0(X_1, X_2, \ldots, X_n)\,.$$

(Alternatively, $I_{r_1,r_2,\ldots,r_n}(X_1, X_2, \ldots, X_n)$ can be obtained from $I^0_{r_1+\ldots+r_n}$ taking the first r_1 arguments to be X_1, then the next r_2 arguments to be X_2 and so on.) Note that the functions $I_{r_1,r_2,\ldots,r_n}$ are everywhere analytic in the n-dimensional complex plane, and invariant under a common permutation of labels r_j and arguments X_j. The basic functions I_n^0 are completely symmetric and they can be obtained from the following recurrence relation

$$I_1^0(X_1) = \mathrm{e}^{X_1}\,, \tag{2.32}$$
$$I_{n+1}^0(X_1, \ldots, X_{n-1}, X_n, X_{n+1}) = \frac{I_n^0(X_1, \ldots, X_{n-1}, X_n) - I_n^0(X_1, \ldots, X_{n-1}, X_{n+1})}{X_n - X_{n+1}}\,.$$

We will use the short-hand notation

$$I_{r_1,r_2,\ldots,r_n} := I_{r_1,r_2,\ldots,r_n}(X_1, X_2, \ldots, X_n)\,. \tag{2.33}$$

With this notation the lowest terms in the derivative expansion are

$$\langle B_0\rangle = \langle I_1\rangle\,,$$
$$\langle B_1\rangle = \left\langle -\frac{1}{2} I_{2,2} X_\mu^2 \right\rangle\,, \tag{2.34}$$
$$\langle B_2\rangle = \Big\langle (-I_{2,2,2,2} + 4I_{3,1,3,1})\,(X_\mu^2)^2 + \frac{1}{2} I_{2,2,2,2}(X_\mu X_\nu)^2 + I_{3,3} X_{\mu\mu}^2 + 4 I_{3,1,3} X_\mu^2 X_{\nu\nu} + 2 I_{2,2,2} X_\mu X_\nu Z_{\mu\nu} + \frac{1}{2} I_{2,2} Z_{\mu\nu}^2 \Big\rangle\,.$$

Expanding in powers of X one obtains for B_2

$$\begin{aligned}\langle B_2\rangle = \Big\langle & \frac{1}{12} Z_{\mu\nu}^2 \\ & + \frac{1}{12} X Z_{\mu\nu}^2 \\ & + \frac{1}{40} X^2 Z_{\mu\nu}^2 + \frac{1}{60} (X Z_{\mu\nu})^2 + \frac{1}{60} X_\mu X_\nu Z_{\mu\nu} \\ & + \frac{1}{120} X_{\mu\mu}^2 \\ & + \frac{1}{180} X^3 Z_{\mu\nu}^2 + \frac{1}{120} X^2 Z_{\mu\nu} X Z_{\mu\nu} \\ & + \frac{1}{180} (X X_\mu X_\nu Z_{\mu\nu} + X_\mu X X_\nu Z_{\mu\nu} X_\mu X_\nu X Z_{\mu\nu}) \\ & + \frac{1}{180} X_\mu^2 X_{\nu\nu} \\ & + \ldots \Big\rangle\,,\end{aligned} \tag{2.35}$$

which reproduces b_2, b_3, b_4, b_5 to four covariant derivatives [17].

The expressions (2.34), together with the similar expression (5.2) for B_3, are the main result of this work. Note that, compared to the standard heat kernel expansion, in the covariant derivative expansion the numerical coefficients of the standard expansion are replaced by coefficients which are functions of labeled X's.

It can be observed that the coefficient functions found are directly consistent with the cyclic property. For instance, the identity

$$\big\langle f(X_1, X_2, X_3, X_4) X_\mu^2 X_\nu^2 \big\rangle = \big\langle f(X_3, X_4, X_1, X_2) X_\nu^2 X_\mu^2 \big\rangle \tag{2.36}$$

shows that one can always choose the coefficient function of $(X_\mu^2)^2$ to be invariant under the cyclic permutation $(X_1, X_2, X_3, X_4) \to (X_3, X_4, X_1, X_2)$ and this symmetry is explicit in $\langle B_2\rangle$ given in (2.34) using the permutation symmetry properties of the functions $I_{r_1,r_2,\ldots,r_n}$.

There is another symmetry also realized in the B_n which will play an important role in what follows. This is *mirror* symmetry, that is, the symmetry under transposition defined by linearity plus the rules

$$(AB)^{\mathrm{T}} = B^{\mathrm{T}} A^{\mathrm{T}}\,, \quad D_\mu^{\mathrm{T}} = D_\mu\,, \quad X^{\mathrm{T}} = X\,. \tag{2.37}$$

They imply $[D_\mu, Y]^{\mathrm{T}} = -[D_\mu, Y^{\mathrm{T}}]$ and thus

$$X^{\mathrm{T}}_{\mu_1\ldots\mu_n} = (-1)^n X_{\mu_1\ldots\mu_n}\,, \quad Z^{\mathrm{T}}_{\mu_1\ldots\mu_n} = (-1)^{n-1} Z_{\mu_1\ldots\mu_n}\,. \tag{2.38}$$

In practice, because the total number of Lorentz indices is always even, an equivalent rule is to pick up a minus sign for each $Z_{\mu_1\ldots\mu_n}$ in the expression.

Mirror symmetry holds for the Klein–Gordon operator K and for the heat kernel e^K, and is manifest in B_0, B_1 and B_2. E.g.

$$\big\langle f(X_1, X_2, X_3) X_\mu^2 X_{\nu\nu}\big\rangle^{\mathrm{T}} = \big\langle f(X_4, X_3, X_2) X_{\nu\nu} X_\mu^2\big\rangle = \big\langle f(X_3, X_2, X_1) X_\mu^2 X_{\nu\nu}\big\rangle \tag{2.39}$$

shows that the coefficient function of $X_\mu^2 X_{\nu\nu}$ (namely, $I_{3,1,3}$ in this case) can be chosen even under transposition of X_1 and X_3. It is curious that the coefficient function of $X_\mu X_\nu Z_{\mu\nu}$ has a greater symmetry than required by cyclic and mirror symmetries.

3 Labeled operators

In this section we describe useful properties of labeled operators. In an expression with labeled operators, there are *fixed operators* relative to which the positions are defined and *labeled operators* which carry position labels, e.g.[5]

$$f(A_1, B_2, C_3, \ldots) X Y \ldots \tag{3.1}$$

X, Y, etc, are the fixed operators in this case, A is to be inserted before (to the left of) X (position 1), B between

[5] The symbols A, B, X, etc, are generic and do not refer to those of the heat kernel throughout this section.

X and Y (position 2), C just after Y (position 3) and so on. Such an expression can be defined in two equivalent ways. First by writing f as a sum of separable functions, e.g.

$$f(x_1,x_2,x_3,\ldots)=\sum_{n_1,n_2,n_3,\ldots} c_{n_1,n_2,n_3,\ldots}x_1^{n_1}x_2^{n_2}x_3^{n_3}\ldots\,,$$
$$f(A_1,B_2,C_3,\ldots)XY\ldots \tag{3.2}$$
$$:=\sum_{n_1,n_2,n_3,\ldots} c_{n_1,n_2,n_3,\ldots}A^{n_1}XB^{n_2}YC^{n_3}\ldots\,.$$

Another example would be the expansion of f as a combination of plane waves, through its Fourier transform.

Alternatively the expression in (3.1) can be interpreted through its matrix elements. Taking $|n,A\rangle$ as a basis of eigenvectors of A with eigenvalue a_n, and similarly for B and C, and $\langle n,A|$, etc. being the corresponding dual basis,

$$\langle n,A|f(A_1,B_2,C_3)XY|r,C\rangle \tag{3.3}$$
$$=\sum_m f(a_n,b_m,c_r)\langle n,A|X|m,B\rangle\langle m,B|Y|r,C\rangle\,.$$

The important point is that the expression in (3.1) depends only on the function f and not on how it is expanded.

The usefulness of the labeled operators stems from the fact that they are effectively c-numbers since e.g. $A_1B_2=B_2A_1$, and so they can be used in several ways. For instance, $[A,\ ]$ can be written as A_1-A_2, since $[A,X]=(A_1-A_2)X$, then $f([A,\ ])$ can be represented as $f(A_1-A_2)$. The well-known identity

$$\mathrm{e}^{[A,\ ]}X=\mathrm{e}^AX\mathrm{e}^{-A} \tag{3.4}$$

becomes trivial using labeled operators

$$\mathrm{e}^{[A,\ ]}X=\mathrm{e}^{A_1-A_2}X=\mathrm{e}^{A_1}\mathrm{e}^{-A_2}X=\mathrm{e}^AX\mathrm{e}^{-A}\,. \tag{3.5}$$

This kind of properties have been used in [33,38] to easily derive commutator expansions.

Labeled operators appear naturally in non-Abelian expansions. If one needs to compute[6] $f(A+B)$ to first order in B, where A and B do not commute, a standard technique is to transform this problem into e^{A+B} by means of a functional transform, and then apply Dyson's formula

$$\mathrm{e}^{A+B}=\mathrm{e}^A+\int_0^1 \mathrm{d}s\,\mathrm{e}^{sA}B\mathrm{e}^{(1-s)A}+O(B^2)\,. \tag{3.6}$$

Using labeled operators one can go further and obtain

$$\mathrm{e}^{A+B}=\mathrm{e}^A+\int_0^1 \mathrm{d}s\mathrm{e}^{sA_1+(1-s)A_2}B+O(B^2)$$
$$=\mathrm{e}^A+\frac{\mathrm{e}^{A_1}-\mathrm{e}^{A_2}}{A_1-A_2}B+O(B^2) \tag{3.7}$$

[6] By $f(A)$, and similar expressions, we mean an ordinary function $f(x)$ evaluated at $x=A$, A being an operator, in the analytical extension sense, as in e^A (and not to completely general operator-valued functions of A). More generally, f may be matrix-valued taking values in a different space than that of A.

(B being the fixed operator). Undoing now the functional transform yields the useful relation, for a generic function $f(x)$,

$$f(A+B)=f(A)+\frac{f(A_1)-f(A_2)}{A_1-A_2}B+O(B^2)\,. \tag{3.8}$$

This relation does not rely on the exponential function and can also be established by using, e.g., a Taylor series expansion of $f(x)$.

From the previous expansion we learn that under a *first order* variation δA of the operator A (the function f being unchanged)

$$\delta\left(f(A)\right)=\nabla f(A_1,A_2)\delta A, \tag{3.9}$$

where the operation ∇ is defined by

$$\nabla f(x_1,x_2):=\frac{f(x_1)-f(x_2)}{x_1-x_2}\,. \tag{3.10}$$

∇ maps a one-argument function $f(x)$ into a two-argument function $\nabla f(x,y)$. Note that δ can be any variation of A, including e.g. a derivative

$$\partial_\mu f(A)=\nabla f(A_1,A_2)\partial_\mu A \tag{3.11}$$

or a commutator, $\delta=[X,\ ]$,

$$[X,f(A)]=\nabla f(A_1,A_2)[X,A] \tag{3.12}$$

(indeed $\nabla f(A_1,A_2)[X,A]=\nabla f(A_1,A_2)(A_2-A_1)X=\left(f(A_2)-f(A_1)\right)X=[X,f(A)]$).

The operator ∇ generalizes the ordinary derivative to the non-Abelian case. Of course, when A and δA commute the right-hand side of (3.9) becomes $f'(A)\delta A$ (applying de l'Hôpital's rule). It is straightforward to verify that the operator ∇ satisfies a Leibniz rule,

$$\nabla(fg)(x_1,x_2)=\nabla f(x_1,x_2)g(x_2)+f(x_1)\nabla g(x_1,x_2)\,, \tag{3.13}$$

where $f(x)$, $g(x)$ are possibly non-commuting (matrix-valued) functions of a single variable. Furthermore, ∇ also complies with the chain rule

$$\nabla(f\circ g)(x_1,x_2)=\nabla f\left(g(x_1),g(x_2)\right)\nabla g(x_1,x_2) \tag{3.14}$$

(in this case $f(x)$ may be matrix valued) as is readily verified.

In the case of several variables one may need partial derivatives, e.g.

$$\delta(f(A_1,B_2)X)$$
$$=\nabla_1 f(A_1,A_2,B_3)\delta A\,X+\nabla_2 f(A_1,B_2,B_3)X\delta B$$
$$+f(A_1,B_2)\delta X\,, \tag{3.15}$$

where ∇_ℓ indicates that it acts on the ℓth argument of f.

It is also convenient to define a ∇ operator acting on the space of functions of any number of variables, in such a way that if maps a n-variable function $f(x_1,\ldots,x_n)$ to a $(n+1)$-variable function, as

$$\nabla:=\sum_k \nabla_k \tag{3.16}$$

(∇_k acting on the kth argument of the function) and so

$$\nabla f(x_1,\dots,x_{n+1}) = \sum_{k=1}^{n} \frac{f(x_1,\dots,\widehat{x_{k+1}},\dots,x_{n+1}) - f(x_1,\dots,\widehat{x_k},\dots,x_{n+1})}{x_k - x_{k+1}}\,, \tag{3.17}$$

where $\widehat{x_\ell}$ indicates that the ℓth argument is missing. The definition is such that

$$\begin{aligned}&\delta\left(f(A_1,\dots,A_n)(\delta A)^{n-1}\right)\\ &\quad= \nabla f(A_1,A_2,\dots,A_{n+1})(\delta A)^n\end{aligned} \tag{3.18}$$

for $\delta(A) = \delta A$ and $\delta(\delta A) = 0$. Using this operator we can write down the non-Abelian version of Taylor's formula

$$f(A+B) = \mathrm{e}^{B\nabla_A} f(A) \tag{3.19}$$

(∇_A emphasizes that ∇ acts on the A-dependence of the expression). That is

$$\begin{aligned}&f(A+B)\\ &= f(A) + \nabla f(A_1,A_2)B + \frac{1}{2!}\nabla^2 f(A_1,A_2,A_3)B^2 + \dots\\ &= f(A) + \frac{f(A_1)-f(A_2)}{A_1-A_2}B\\ &\quad + \left(\frac{f(A_1)}{(A_2-A_1)(A_3-A_1)} + \frac{f(A_2)}{(A_1-A_2)(A_3-A_2)}\right.\\ &\qquad \left. + \frac{f(A_3)}{(A_1-A_3)(A_2-A_3)}\right)B^2 + \dots\,.\end{aligned} \tag{3.20}$$

In the Abelian case the coefficients reduce to those of the standard Taylor expansion.

To finish this section we note a very important point when using labeled operators, namely, that of the regularity of the functions of the type $f(A_1,A_2,\dots)$ at the coincidence limit of two or more arguments. These functions must be regular (free from poles) at the coincidence limit to define meaningful operators. For instance, an expression of the type

$$\frac{1}{A_1-A_2}B \tag{3.21}$$

is only formal as it refers to any solution Y of the equation $[A,Y] = B$. Depending on the operators A and B such a solution either does not exist or is not unique. The operation ∇ (cf. (3.10)) does not introduce singularities (poles) in that limit and the functions appearing in the expansion (3.20) are all regular.

4 Diagonal heat kernel coefficients

The diagonal coefficients $A_n(x)$ can be computed using e.g. the method of symbols, however, having the B_n it is simpler to derive them from the relation [6]

$$\delta_X \operatorname{Tr} \mathrm{e}^{D_\mu^2 + X} = \operatorname{Tr}\left(\mathrm{e}^{D_\mu^2+X}\delta X\right), \tag{4.1}$$

where δ_X is a first order variation with respect to X. That is

$$\langle x|\mathrm{e}^K|x\rangle = \frac{\delta \operatorname{Tr}\mathrm{e}^K}{\delta X(x)}\,. \tag{4.2}$$

For the Seeley–DeWitt coefficients this implies

$$a_n(x) = (4\pi)^{d/2}\frac{\delta\langle b_{n+1}\rangle}{\delta X(x)}\,, \tag{4.3}$$

whereas for the derivative expansion coefficients it gives

$$A_n(x) = (4\pi)^{d/2}\frac{\delta\langle B_n\rangle}{\delta X(x)}\,. \tag{4.4}$$

This relation allows one to obtain A_n from B_n, but B_n can also be obtained from A_n through (2.10). This implies the consistency condition

$$\langle B_n\rangle = (4\pi)^{d/2}\left\langle\frac{\delta\langle B_n\rangle}{\delta X(x)}\right\rangle. \tag{4.5}$$

It can be shown that this consistency condition is satisfied by our expressions (2.34). This only requires the property

$$I_{r_1,r_2,\dots,r_n} = \mathrm{e}^{X_1} f(X_2-X_1,\dots,X_n-X_1) \tag{4.6}$$

(this relation codifies the heat kernel property $\mathrm{e}^K \to \mathrm{e}^a\mathrm{e}^K$ under the shift $X \to X+a$, a being a c-number). The consistency condition is not sufficient to determine B_n since it will be satisfied too by all heat kernel-like operators of the form $\exp\left(X + f(D_\mu^2)\right)$.

Using the results in Sect. 3 relative to the manipulation of labeled operators, one can carry out the functional derivative with respect to X indicated in (4.4) for $\langle B_n\rangle$ given in (2.34). However, in the present case it is simpler to go back to F_n (i.e., before integration over z and labeling of operators) and do the variation there, using the identity

$$\delta_X N = N\delta X N\,. \tag{4.7}$$

We illustrate the method with A_1:

$$\begin{aligned}&\delta_X\langle F_1\rangle\\ &= \delta_X\left\langle\frac{1}{2}N^2X_\mu N^2X_\mu\right\rangle\\ &= \big\langle N\delta X N^2X_\mu N^2X_\mu + N^2\delta X N X_\mu N^2X_\mu\\ &\qquad + N^2(\delta X)_\mu N^2X_\mu\big\rangle\\ &= \big\langle\big(N^2X_\mu N^2X_\mu N + NX_\mu N^2X_\mu N^2\\ &\qquad -(N^2X_\mu N^2)_\mu\big)\,\delta X\big\rangle\\ &= \big\langle\big(-2N^2X_\mu N X_\mu N^2 - N^2X_{\mu\mu}N^2\big)\delta X\big\rangle\,.\end{aligned} \tag{4.8}$$

I.e.

$$\frac{\delta\langle F_1\rangle}{\delta X} = -\frac{1}{(4\pi)^{d/2}}\left(2N_1^2N_2N_3^2X_\mu X_\mu + N_1^2N_2^2X_{\mu\mu}\right). \tag{4.9}$$

Following the same procedure with F_2 and carrying out the integration over z, we find

$$
\begin{aligned}
A_0 &= I_1\,,\\
A_1 &= 2I_{2,1,2}X_\mu^2 + I_{2,2}X_{\mu\mu}\,,\\
A_2 &= 2I_{2,1,2}\,Z_{\mu\nu}Z_{\mu\nu}\\
&+ (4I_{2,2,2} - 8I_{3,0,3} + 8I_{2,1,3})\,Z_{\mu\mu\nu}X_\nu\\
&+ (4I_{2,1,2,2} - 16I_{3,0,1,3})\,X_\mu Z_{\mu\nu}X_\nu\\
&+ (32I_{3,0,1,3} - 16I_{2,1,1,3} - 8I_{2,1,2,2} + 16I_{3,0,2,2})\,Z_{\mu\nu}X_\mu X_\nu\\
&+ 2I_{3,3}\,X_{\mu\mu\nu\nu}\\
&+ (2I_{2,3,2} + 4I_{3,1,3} + 4I_{2,2,3})\,X_{\mu\mu}X_{\nu\nu}\\
&+ 8I_{3,1,3}\,X_{\mu\nu}X_{\mu\nu}\\
&+ (16I_{3,1,3} + 8I_{3,2,2})\,X_{\mu\nu\nu}X_\mu\\
&+ (4I_{2,2,2,2} + 16I_{3,1,1,3} + 16I_{2,2,1,3})\,X_\mu X_{\mu\nu}X_\nu\\
&+ (2I_{2,2,2,2} + 8I_{3,1,1,3} + 8I_{2,2,1,3})\,X_\mu X_{\nu\nu}X_\mu\\
&+ (4I_{2,2,2,2} + 16I_{3,1,1,3} + 8I_{2,2,1,3} + 8I_{2,3,1,2} + 8I_{3,1,2,2}\\
&\quad +8I_{3,2,1,2})\,X_{\mu\mu}X_\nu X_\nu\\
&+ (32I_{3,1,1,3} + 16I_{3,1,2,2})\,X_{\mu\nu}X_\mu X_\nu\\
&+ (4I_{2,2,1,2,2} + 16I_{3,1,1,1,3} + 16I_{2,1,2,1,3} + 8I_{2,2,2,1,2}\\
&\quad +8I_{2,1,3,1,2} + 16I_{2,2,1,1,3})\,X_\mu X_\mu X_\nu X_\nu \qquad (4.10)\\
&+ (4I_{2,2,1,2,2} + 16I_{3,1,1,1,3} + 16I_{2,2,1,1,3})\,X_\mu X_\nu X_\mu X_\nu\\
&+ (4I_{2,2,1,2,2} + 16I_{3,1,1,1,3} + 16I_{2,2,1,1,3})\,X_\mu X_\nu X_\nu X_\mu\,.
\end{aligned}
$$

A_1 is a direct transcription of (4.8). However, in A_2 we have shortened the expression by using a standard convention, namely, we have identified every term with its mirror conjugate and have used only one of the two forms. In other words, each term stands for the semi sum of itself plus its mirror conjugate. For instance,

$$
\begin{aligned}
&4I_{2,2,3}\,X_{\mu\mu}X_{\nu\nu} := (2I_{2,2,3} + 2I_{3,2,2})\,X_{\mu\mu}X_{\nu\nu}\,,\\
&16I_{3,0,2,2}\,Z_{\mu\nu}X_\mu X_\nu\\
&\quad := 8I_{3,0,2,2}\,Z_{\mu\nu}X_\mu X_\nu + 8I_{2,2,0,3}\,X_\mu X_\nu Z_{\mu\nu}\,. \qquad (4.11)
\end{aligned}
$$

In obtaining A_2 we have used the Jacobi identity (here Y represents an arbitrary quantity)

$$Y_{\mu\nu} = Y_{\nu\mu} + [Z_{\mu\nu}, Y] \qquad (4.12)$$

to reduce the number of terms, e.g. by eliminating terms of the type $X_{\mu\nu}Z_{\mu\nu}$ (as $\frac{1}{2}[Z_{\mu\nu}, X]Z_{\mu\nu}$) and by canonically ordering the Lorentz indices.

5 Six derivative terms, B_3

The term F_3 in the expansion (2.15) has been computed in [39]:

$$
\begin{aligned}
F_3 = &+\frac{20}{3}N_\alpha N_\alpha N_\beta N_\beta N_\gamma N_\gamma - 2N_\alpha N_\beta N_\alpha N_\gamma N_\beta N_\gamma\\
&+\frac{2}{3}N_\alpha N_\beta N_\gamma N_\alpha N_\beta N_\gamma + 2N_\alpha N_\alpha N_\beta N_\gamma N_\gamma N_\beta\\
&-4N_\alpha N_\alpha N_\beta N_\gamma N_\beta N_\gamma - 16NN_\alpha N_\beta N_\alpha N_\gamma N_{\beta\gamma}\\
&+16NN_\alpha N_\beta N_\beta N_\gamma N_{\alpha\gamma} + 6N^2N_{\alpha\alpha}N_\beta N_\beta N_{\gamma\gamma}\\
&-16NN_{\alpha\alpha}NN_{\beta\beta}N_\gamma N_\gamma - 8NN_\alpha N_{\alpha\beta}NN_\gamma N_{\gamma\beta}\\
&-16NN_\alpha N_{\alpha\beta}N_\beta NN_{\gamma\gamma} - 8NN_\alpha N_\beta NN_{\alpha\gamma}N_{\beta\gamma}\\
&+8NN_\alpha N_\beta NN_{\beta\gamma}N_{\alpha\gamma} + 10NN_\alpha N_{\beta\beta}NN_\alpha N_{\gamma\gamma}\\
&-4NN_\alpha N_{\beta\beta}NN_{\gamma\gamma}N_\alpha + 8NN_\alpha N_{\beta\beta}N_\alpha NN_{\gamma\gamma}\\
&-\frac{8}{3}NN_{\alpha\alpha}NN_{\beta\beta}NN_{\gamma\gamma} + 12N^2N_{\alpha\alpha}N_\beta NN_{\beta\gamma\gamma}\\
&+3N^2N_{\alpha\beta\beta}N^2N_{\alpha\gamma\gamma} - 8Z_{\alpha\beta}N_\gamma NN_\alpha N_\beta NN_\gamma\\
&+4NZ_{\alpha\beta}NN_\gamma N_\alpha N_\beta N_\gamma - 8NZ_{\alpha\beta}NN_\alpha N_\beta N_\gamma N_\gamma\\
&-8NZ_{\alpha\beta}NN_\alpha N_\gamma N_\beta N_\gamma - 4NZ_{\alpha\beta}NN_\alpha N_\gamma N_\gamma N_\beta\\
&-16NZ_{\alpha\beta}NN_\alpha NN_{\gamma\gamma}N_\beta - 16Z_{\alpha\beta}N^2N_{\gamma\gamma}NN_\alpha N_\beta\\
&-16Z_{\alpha\beta}N^2N_\gamma N_{\gamma\alpha}NN_\beta - 16NZ_{\alpha\beta}N^2N_{\alpha\gamma}N_\gamma N_\beta\\
&-16NZ_{\alpha\beta}N^2N_\alpha N_{\gamma\gamma}N_\beta - 8N^2Z_{\alpha\beta}N^2N_{\alpha\gamma}N_{\beta\gamma}\\
&-16N^2Z_{\alpha\beta}N^2N_\alpha N_{\beta\gamma\gamma} - 16NZ_{\alpha\beta}N^2N_{\alpha\gamma\gamma}NN_\beta\\
&+8N^2Z_{\alpha\alpha\beta}N^2N_\beta N_{\gamma\gamma} - 2N^3Z_{\alpha\alpha\beta}N^3Z_{\gamma\beta\gamma}\\
&+16Z_{\alpha\beta}N^3Z_{\gamma\alpha\gamma}N^2N_\beta + NZ_{\alpha\beta}NN_\gamma NZ_{\alpha\beta}NN_\gamma\\
&-4NZ_{\alpha\beta}NN_\alpha NZ_{\beta\gamma}NN_\gamma - 4N^2Z_{\alpha\beta}N^2N_\gamma Z_{\alpha\beta}N_\gamma\\
&+8Z_{\alpha\beta}N^2N_\gamma Z_{\alpha\gamma}N^2N_\beta + 16Z_{\alpha\beta}N^3Z_{\alpha\gamma}N_\gamma NN_\beta\\
&-2NZ_{\alpha\beta}N^2Z_{\alpha\beta}NN_\gamma N_\gamma - 4NZ_{\alpha\beta}N^2Z_{\alpha\gamma}NN_\beta N_\gamma\\
&+4NZ_{\alpha\beta}N^2Z_{\alpha\gamma}NN_\gamma N_\beta - 8Z_{\alpha\beta}N^3Z_{\alpha\beta}N^2N_{\gamma\gamma}\\
&-\frac{4}{3}N^2Z_{\alpha\beta}N^2Z_{\alpha\gamma}N^2Z_{\beta\gamma}\,. \qquad (5.1)
\end{aligned}
$$

In this formula the number of explicit terms has been reduced by identifying terms related by
(i) cyclic permutations and
(ii) mirror symmetry. As noted before some conventions here differ from those in [39]. In order to obtain the heat kernel coefficient B_3 from F_3 we use the procedure of Sect. 2, as in e.g. (2.28). This yields

$$
\begin{aligned}
\langle B_3\rangle = \Big\langle &-3I_{44}X_{\alpha\beta\beta}X_{\alpha\gamma\gamma} - 24I_{414}X_\alpha X_{\beta\alpha}X_{\beta\gamma\gamma}\\
&+(-12I_{324} - 12I_{414})X_\alpha X_{\beta\beta}X_{\alpha\gamma\gamma} + \frac{8}{3}I_{333}X_{\alpha\alpha}X_{\beta\beta}X_{\gamma\gamma}\\
&+(-24I_{4114} - 24I_{4123})X_\alpha X_\alpha X_\beta X_{\beta\gamma\gamma}\\
&-12I_{4114}X_\alpha X_\beta X_\alpha X_{\beta\gamma\gamma}\\
&+(-12I_{1324} - 6I_{1414} - 6I_{2224} + 16I_{2233} + 4I_{2323}\\
&\quad +16I_{3133})X_\alpha X_\alpha X_{\beta\beta}X_{\gamma\gamma}\\
&+(-24I_{1414} - 24I_{2314})X_\alpha X_\beta X_{\alpha\beta}X_{\gamma\gamma}\\
&+8I_{3232}X_\alpha X_\beta X_{\alpha\gamma}X_{\beta\gamma} - 8I_{3232}X_\alpha X_\beta X_{\beta\gamma}X_{\alpha\gamma}
\end{aligned}
$$

$$
\begin{aligned}
&- 24I_{1414}X_\alpha X_\beta X_{\gamma\beta}X_{\gamma\alpha}\\
&+ (-24I_{1414} - 24I_{2314} + 16I_{3223})X_\alpha X_{\alpha\beta}X_\beta X_{\gamma\gamma}\\
&+ 8I_{3232}X_\alpha X_{\alpha\beta}X_\gamma X_{\gamma\beta} - 24I_{4141}X_\alpha X_{\beta\alpha}X_\gamma X_{\beta\gamma}\\
&+ (-6I_{1414} - 12I_{1423} - 10I_{2323} - 8I_{2332})X_\alpha X_{\beta\beta}X_\alpha X_{\gamma\gamma}\\
&+ (-24I_{13214} - 24I_{14114} - 24I_{22214} + 32I_{22313} - 24I_{23114}\\
&\quad +16I_{23213} + 32I_{31223} + 32I_{31313}\\
&\qquad +16I_{32123})X_\alpha X_\alpha X_\beta X_\beta X_{\gamma\gamma}\\
&+ (-48I_{41141} - 48I_{41231})X_\alpha X_\alpha X_\beta X_\gamma X_{\beta\gamma}\\
&+ 16I_{32132}X_\alpha X_\alpha X_\beta X_\gamma X_{\gamma\beta}\\
&+ (-16I_{13232} - 16I_{22232} + 32I_{31322} - 48I_{41141}\\
&\qquad -48I_{41231})X_\alpha X_\alpha X_\beta X_{\beta\gamma}X_\gamma\\
&+ (-24I_{11324} - 24I_{11414} - 16I_{21233} - 40I_{21323} - 24I_{21413}\\
&\qquad -16I_{31322})X_\alpha X_\alpha X_\beta X_{\gamma\gamma}X_\beta\\
&+ (-24I_{14114} - 24I_{23114} + 16I_{32123})X_\alpha X_\beta X_\alpha X_\beta X_{\gamma\gamma}\\
&+ (16I_{32222} + 16I_{32312} - 48I_{41141})X_\alpha X_\beta X_\alpha X_\gamma X_{\beta\gamma}\\
&+ (-16I_{21323} + 16I_{32132})X_\alpha X_\beta X_\alpha X_\gamma X_{\gamma\beta}\\
&+ 16I_{32312}X_\alpha X_\beta X_\gamma X_\alpha X_{\beta\gamma}\\
&+ (-24I_{114114} - 48I_{114123} - 8I_{121323} - 16I_{122223}\\
&\quad +32I_{123132} + 16I_{213123} + 64I_{213132} - 24I_{214122}\\
&\qquad -\frac{20}{3}I_{222222} + \frac{64}{3}I_{313131}\Big)X_\alpha X_\alpha X_\beta X_\beta X_\gamma X_\gamma\\
&+ (-48I_{114114} + 8I_{121323} + 16I_{122223} + 16I_{123123}\\
&\quad -16I_{132312} - 48I_{214113} - 16I_{222213}\\
&\qquad +4I_{222222} + 32I_{313212})X_\alpha X_\alpha X_\beta X_\gamma X_\beta X_\gamma\\
&+ (-48I_{113214} - 24I_{114114} + 8I_{123123} - 32I_{212313}\\
&\qquad -40I_{213213} - 2I_{222222})X_\alpha X_\alpha X_\beta X_\gamma X_\gamma X_\beta\\
&+ (16I_{121323} - 8I_{213231} + 16I_{221322} + 2I_{222222}\\
&\qquad +8I_{312312} - 12I_{411411})X_\alpha X_\beta X_\alpha X_\gamma X_\beta X_\gamma\\
&+ \left(8I_{121323} - \frac{2}{3}I_{222222}\right)X_\alpha X_\beta X_\gamma X_\alpha X_\beta X_\gamma\\
&+ 8I_{323}X_\alpha X_{\beta\beta}Z_{\gamma\alpha\gamma} + (16I_{233} + 16I_{323})X_\alpha X_{\beta\gamma\gamma}Z_{\alpha\beta}\\
&+ 8I_{323}X_{\alpha\beta}X_{\gamma\beta}Z_{\alpha\gamma}\\
&- 16I_{3123}X_\alpha X_\alpha X_\beta Z_{\gamma\beta\gamma} + 16I_{3123}X_\alpha X_\beta X_{\gamma\alpha}Z_{\beta\gamma}\\
&+ 16I_{3231}X_\alpha X_{\alpha\beta}X_\gamma Z_{\beta\gamma}\\
&+ (16I_{2223} + 32I_{2313} + 16I_{3123} + 32I_{3213})X_\alpha X_\beta X_{\gamma\beta}Z_{\alpha\gamma}\\
&+ (16I_{1233} + 16I_{2313} + 16I_{3213})X_\alpha X_\beta X_{\gamma\gamma}Z_{\alpha\beta}\\
&+ (32I_{3123} + 32I_{3132})X_\alpha X_{\beta\alpha}X_\gamma Z_{\beta\gamma}\\
&+ (16I_{2223} + 16I_{2232} + 16I_{2313}\\
&\qquad +16I_{3123})X_\alpha X_{\beta\beta}X_\gamma Z_{\alpha\gamma}\\
&+ (8I_{22222} + 32I_{31123} + 32I_{31132} + 32I_{31321}\\
&\qquad +16I_{32131})X_\alpha X_\alpha X_\beta X_\gamma Z_{\beta\gamma}\\
&+ (8I_{22222} + 32I_{31123} + 32I_{31132} + 16I_{31213} + 16I_{31222}\\
&\qquad +16I_{32131})X_\alpha X_\beta X_\alpha X_\gamma Z_{\beta\gamma}\\
&+ (32I_{22123} + 32I_{22132} + 16I_{22213} + 4I_{22222} + 32I_{23113}\\
&\qquad +32I_{31123} + 8I_{31213})X_\alpha X_\beta X_\beta X_\gamma Z_{\alpha\gamma}\\
&+ (8I_{13231} - 4I_{22222} + 8I_{31213})X_\alpha X_\beta X_\gamma X_\alpha Z_{\beta\gamma}\\
&+ 2I_{33}Z_{\alpha\alpha\beta}Z_{\gamma\beta\gamma} + 16I_{313}X_\alpha Z_{\alpha\beta}Z_{\gamma\beta\gamma}\\
&+ 8I_{133}X_{\alpha\alpha}Z_{\beta\gamma}Z_{\beta\gamma} + (16I_{1133} + 2I_{2222})X_\alpha X_\alpha Z_{\beta\gamma}Z_{\beta\gamma}\\
&+ 4I_{2222}X_\alpha X_\beta Z_{\alpha\gamma}Z_{\beta\gamma}\\
&+ (-16I_{1313} - 4I_{2222})X_\alpha X_\beta Z_{\beta\gamma}Z_{\alpha\gamma}\\
&+ (4I_{2222} + 8I_{3131})X_\alpha Z_{\alpha\beta}X_\gamma Z_{\beta\gamma}\\
&+ (4I_{1331} - I_{2222})X_\alpha Z_{\beta\gamma}X_\alpha Z_{\beta\gamma} + \frac{4}{3}I_{222}Z_{\alpha\beta}Z_{\alpha\gamma}Z_{\beta\gamma}\Big\rangle .
\end{aligned}
\tag{5.2}
$$

For the proper interpretation of this formula, it is important to recall that mirror symmetric terms have been identified, as in (4.11).

F_3 contains 45 terms but only 40 different structures of fixed operators, since some of the terms differ only by the position of underivated N's. Similarly, B_3 contains 52 different *structures* of fixed operators (e.g. $X_\alpha Z_{\beta\gamma}X_\alpha Z_{\beta\gamma}$), each with a coefficient function written as a combination of functions $I_{r_1,r_2,\ldots,r_n}$. Counting each of these as different, B_3 contains a total of 147 *terms*.

As explained at length in [39], the expression of F_3 is not unique due to integration by parts and the Jacobi identity (4.12) and this is also true for B_3. The previous expression for B_3 comes directly from F_3 using only cyclic and mirror symmetries to reduce the number of terms. This is also the shortest expression we have found for B_3 from the point of view of the number of terms. No systematic minimization of the number of terms in B_3 has been attempted (it was done in [39] for F_3), nevertheless the existence of a much shorter expression seems unlikely. Alternatively, one can try to reduce the number of structures. The length defined from the point of view of the number of structures can be reduced from 52 to 37. This is because, as discussed below, all functionals of the type of B_3 can be written using a standard basis of structures with 37 elements. (Conceivably, a concrete functional such as B_3 could be written using a smaller number of structures, but this is unlikely.) The price to pay for a smaller number of structures is to increase the number of terms from 147 to about two thousand terms.

6 Basis of structures with two, four and six derivatives

Instead of finding shortest expressions, it is also of interest to find a standard basis [40, 41] of structures. We discuss that problem in this section.

Specifically, one would like to express a generic gauge invariant functional $F(D,X)$ constructed with D_μ and X and with a fixed number of covariant derivatives, as a combination of structures T_i (the basis, independent of the functional F) with F-dependent coefficients $F^{(i)}$ which are functions of labeled X's:

$$\langle F\rangle = \sum_{i=1}^{N} \left\langle F^{(i)}(X_1,X_2,\ldots)T_i\right\rangle \tag{6.1}$$

(the number of arguments in $F^{(i)}$ being the number of fixed operators in the structure T_i).

A standard basis is subject to some requirements, namely,
(i) the structures in the basis must be sufficient to express any functional and
(ii) all of them must be necessary (i.e., no one can be removed from the basis without spoiling the requirement (i)).

The expressions for B_0, B_1 and B_2 in (2.34) suggest that the following are standard basis for gauge invariant functionals with cyclic and mirror symmetry: For zero derivatives,

$$T_1 = 1\,. \tag{6.2}$$

For functionals with two derivatives

$$T_1 = X_\mu^2\,, \tag{6.3}$$

and for four covariant derivatives,

$$\begin{aligned} &T_1 = (X_\mu^2)^2, \quad T_2 = (X_\mu X_\nu)^2, \quad T_3 = X_{\mu\mu}^2,\\ &T_4 = X_\mu^2 X_{\nu\nu}, \quad T_5 = X_\mu X_\nu Z_{\mu\nu}, \quad T_6 = Z_{\mu\nu}^2. \end{aligned} \tag{6.4}$$

This is indeed so. For instance, for two covariant derivatives, in addition to $T_1 = X_\mu^2$, one could write down a further structure $X_{\mu\mu}$, however, this is redundant since

$$\begin{aligned} &\langle f(X)\, X_{\mu\mu}\rangle\\ &= \langle -[D_\mu, f(X)]\, X_\mu\rangle = \left\langle -\nabla f(X_1,X_2)\, X_\mu^2\right\rangle\\ &= \left\langle F^{(1)}(X_1,X_2)\, T_1\right\rangle\,. \end{aligned} \tag{6.5}$$

As we have noted at the end of Sect. 3 the coefficient functions $F^{(i)}(X_1,X_2,\ldots)$ must be regular in the coincidence limit of two or more arguments to define meaningful expressions. If this requirement is not met one finds that formally a smaller number of structures would suffice. For four derivatives these are T_1 and T_2. For instance, T_3 can be reduced to T_1 as follows:

$$\begin{aligned} &\left\langle f(X_1,X_2)X_{\mu\mu}^2\right\rangle\\ &= \langle f(X_1,X_3)(X_1-2X_2+X_3)(X_3-2X_4+X_1)\\ &\quad \times D_\mu D_\mu D_\nu D_\nu\rangle\\ &= \Big\langle f(X_1,X_3)\\ &\quad \times \frac{(X_1-2X_2+X_3)(X_3-2X_4+X_1)}{(X_2-X_1)(X_3-X_2)(X_4-X_3)(X_1-X_4)}\\ &\quad \times X_\mu X_\mu X_\nu X_\nu\Big\rangle\\ &= \left\langle F^{(1)}(X_1,X_2,X_3,X_4)\, T_1\right\rangle\,. \end{aligned} \tag{6.6}$$

Such a reduction is faulty as the identity used in the second step $D_\mu \to (X_2-X_1)^{-1}X_\mu$ is only formal (as noted above, the equation $[Y,X]=X_\mu$ does not imply $Y=D_\mu$).

In addition to being sufficient and necessary, for a standard basis one may ask whether the coefficients $F^{(i)}$ are unique. In general they will not be unique. For instance, for the structure X_μ^2, to any given $F^{(1)}(X_1,X_2)$, one can add an arbitrary odd function $f(X_1,X_2) = -f(X_2,X_1)$. Such an addition $\left\langle f(X_1,X_2)X_\mu^2\right\rangle$ vanishes identically using cyclic symmetry. Therefore, $F^{(1)}(X_1,X_2)$ can only be unique if one imposes the further condition that it must be symmetric under transposition of X_1 and X_2. It is clear that under such restriction $F^{(1)}(X_1,X_2)$ is unique. (This can be verified using the technique of bare structures introduced below.) Equivalently, a functional $\left\langle F^{(1)}(X_1,X_2)X_\mu^2\right\rangle$ is identically zero if and only if the symmetric function $F^{(1)}(X_1,X_2)$ is identically zero.

In the four derivative case, the coefficients can always be chosen to have the following symmetries

$$\begin{aligned} &F^{(1)}_{1234} = F^{(1)}_{1432} = F^{(1)}_{3214} = F^{(1)}_{3412}\,,\\ &F^{(2)}_{1234} = F^{(2)}_{1432} = F^{(2)}_{2143} = F^{(2)}_{2341} = F^{(2)}_{3214} = F^{(2)}_{3412}\\ &\qquad = F^{(2)}_{4123} = F^{(2)}_{4321}\,,\\ &F^{(3)}_{12} = F^{(3)}_{21}\,,\\ &F^{(4)}_{123} = F^{(4)}_{321}\,,\\ &F^{(5)}_{123} = F^{(5)}_{321}\,,\\ &F^{(6)}_{12} = F^{(6)}_{21}\,, \end{aligned} \tag{6.7}$$

where we use a shorthand notation e.g. $F^{(2)}_{1432} = F^{(2)}(X_1, X_4, X_3, X_2)$. For instance

$$\begin{aligned} &\left\langle F^{(5)}_{123} X_\mu X_\nu Z_{\mu\nu}\right\rangle\\ &= -\left\langle F^{(5)}_{432} Z_{\mu\nu} X_\nu X_\mu\right\rangle = -\left\langle F^{(5)}_{321} X_\nu X_\mu Z_{\mu\nu}\right\rangle\\ &= \left\langle F^{(5)}_{321} X_\mu X_\nu Z_{\mu\nu}\right\rangle \end{aligned} \tag{6.8}$$

(using, in the first equality, that a term and its mirror symmetric have been identified). With these symmetry restrictions, these $F^{(i)}$ can be shown to be unique.

We finally come to the six derivative case (always assuming gauge invariant functionals with cyclic and mirror symmetries). The 52 structures appearing for B_3 in (5.2) are neither necessary nor sufficient. A standard basis is as follows:

$$\begin{aligned} &T_1 = X_{\alpha\beta\gamma}X_{\alpha\beta\gamma}\,, \quad T_2 = X_\alpha X_{\beta\gamma}X_{\alpha\beta\gamma}\,,\\ &T_3 = X_{\alpha\beta}X_{\alpha\gamma}X_{\beta\gamma}\,, \quad T_4 = X_\alpha X_\alpha X_{\beta\gamma}X_{\beta\gamma}\,, \end{aligned}$$

$$
\begin{aligned}
&T_5 = X_\alpha X_\beta X_\gamma X_{\alpha\beta\gamma}\,, \quad T_6 = X_\alpha X_\beta X_{\alpha\gamma} X_{\beta\gamma}\,,\\
&T_7 = X_\alpha X_\beta X_{\beta\gamma} X_{\alpha\gamma}\,, \quad T_8 = X_\alpha X_{\alpha\beta} X_\gamma X_{\gamma\beta}\,,\\
&T_9 = X_\alpha X_{\beta\gamma} X_\alpha X_{\beta\gamma}\,, \quad T_{10} = X_\alpha X_\alpha X_\beta X_\gamma X_{\beta\gamma}\,,\\
&T_{11} = X_\alpha X_\beta X_\beta X_\gamma X_{\alpha\gamma}\,, \quad T_{12} = X_\alpha X_\beta X_\alpha X_\gamma X_{\beta\gamma}\,,\\
&T_{13} = X_\alpha X_\beta X_\gamma X_\alpha X_{\beta\gamma}\,, \quad T_{14} = X_\alpha X_\alpha X_\beta X_\beta X_\gamma X_\gamma\,,\\
&T_{15} = X_\alpha X_\alpha X_\beta X_\gamma X_\beta X_\gamma\,, \quad T_{16} = X_\alpha X_\alpha X_\beta X_\gamma X_\gamma X_\beta\,,\\
&T_{17} = X_\alpha X_\beta X_\alpha X_\gamma X_\beta X_\gamma\,, \quad T_{18} = X_\alpha X_\beta X_\gamma X_\alpha X_\beta X_\gamma\,,\\
&T_{19} = X_\alpha X_{\beta\gamma} Z_{\beta\alpha\gamma}\,, \quad T_{20} = X_{\alpha\beta} X_{\alpha\gamma} Z_{\beta\gamma}\,,\\
&T_{21} = X_\alpha X_\beta X_\gamma Z_{\alpha\beta\gamma}\,, \quad T_{22} = X_\alpha X_\beta X_{\alpha\gamma} Z_{\beta\gamma}\,,\\
&T_{23} = X_\alpha X_\beta X_{\beta\gamma} Z_{\alpha\gamma}\,, \quad T_{24} = X_\alpha X_{\alpha\beta} X_\gamma Z_{\beta\gamma}\,,\\
&T_{25} = X_\alpha X_\alpha X_\beta X_\gamma Z_{\beta\gamma}\,, \quad T_{26} = X_\alpha X_\beta X_\alpha X_\gamma Z_{\beta\gamma}\,,\\
&T_{27} = X_\alpha X_\beta X_\beta X_\gamma Z_{\alpha\gamma}\,, \quad T_{28} = X_\alpha X_\beta X_\gamma X_\alpha Z_{\beta\gamma}\,,\\
&T_{29} = Z_{\alpha\beta\gamma} Z_{\alpha\beta\gamma}\,, \quad T_{30} = X_\alpha Z_{\beta\gamma} Z_{\alpha\beta\gamma}\,,\\
&T_{31} = X_{\alpha\beta} Z_{\alpha\gamma} Z_{\beta\gamma}\,, \quad T_{32} = X_\alpha X_\alpha Z_{\beta\gamma} Z_{\beta\gamma}\,,\\
&T_{33} = X_\alpha X_\beta Z_{\alpha\gamma} Z_{\beta\gamma}\,, \quad T_{34} = X_\alpha X_\beta Z_{\beta\gamma} Z_{\alpha\gamma}\,,\\
&T_{35} = X_\alpha Z_{\alpha\beta} X_\gamma Z_{\beta\gamma}\,, \quad T_{36} = X_\alpha Z_{\beta\gamma} X_\alpha Z_{\beta\gamma}\,,\\
&T_{37} = Z_{\alpha\beta} Z_{\alpha\gamma} Z_{\beta\gamma}\,. \qquad (6.9)
\end{aligned}
$$

To establish that this set is sufficient we follow the ideas put forward by Müller in [41] for the standard heat kernel expansion. Consider the set of all possible structures with six derivatives, removing those that are redundant using
(i) dummy indices,
(ii) cyclic symmetry and
(iii) mirror symmetry.

There are 211 such distinct structures. Using integration by parts one can always remove all structures where Lorentz indices are contracted within the same factor, e.g. the index α in $X_{\alpha\alpha} X_{\beta\gamma} X_{\beta\gamma}$. Next, one can use the Jacobi identity (4.12) to choose the order of the covariant derivatives within each factor, for instance, if $X_{\alpha\beta\gamma} X_{\alpha\beta\gamma}$ is retained, $X_{\alpha\beta\gamma} X_{\alpha\gamma\beta}$ becomes redundant. For the same reason all structures of the type $(\ldots Y_{\ldots\alpha\beta\ldots\gamma} \ldots Z_{\ldots\alpha\beta})$ are also redundant. Finally, $X_\alpha X_\beta X_\gamma Z_{\beta\alpha\gamma}$ can be reduced to T_{21} using the Bianchi identity

$$
Z_{\alpha\beta\gamma} = Z_{\beta\alpha\gamma} + Z_{\gamma\beta\alpha}\,. \qquad (6.10)
$$

This produces the set of structures in (6.9).

The above constructive procedure shows that the 37 structures are sufficient. Before showing that they are also necessary, we need to discuss the symmetries of their coefficient functions $F^{(i)}$. These are as follows:

$$
\begin{aligned}
&F^{(1)}_{12} = F^{(1)}_{21}\,, \quad F^{(3)}_{123} = F^{(3)}_{213} = F^{(3)}_{321}\,, \quad F^{(4)}_{1234} = F^{(4)}_{3214},\\
&F^{(5)}_{1234} = F^{(5)}_{4321}\,, \quad F^{(6)}_{1234} = F^{(6)}_{3214}\,, \quad F^{(7)}_{1234} = F^{(7)}_{3214},\\
&F^{(8)}_{1234} = F^{(8)}_{3412}\,, \quad F^{(9)}_{1234} = F^{(9)}_{2143} = F^{(9)}_{3412},\\
&F^{(11)}_{12345} = F^{(11)}_{32154}\,, \quad F^{(13)}_{12345} = F^{(13)}_{54321}\,,\\
&F^{(14)}_{123456} = F^{(14)}_{165432} = F^{(14)}_{321654}\,, \quad F^{(15)}_{123456} = F^{(15)}_{321654}\,,\\
&F^{(16)}_{123456} = F^{(16)}_{321654} = F^{(16)}_{456123}\,,\\
&F^{(17)}_{123456} = F^{(17)}_{165432} = F^{(17)}_{456123}\,,\\
&F^{(18)}_{123456} = F^{(18)}_{654321} = F^{(18)}_{234561}\,,\\
&F^{(20)}_{123} = F^{(20)}_{321}\,, \quad F^{(27)}_{12345} = F^{(27)}_{54321}\,, \quad F^{(28)}_{12345} = F^{(28)}_{54321}\,,\\
&F^{(29)}_{12} = F^{(29)}_{21}\,, \quad F^{(31)}_{123} = F^{(31)}_{213}\,, \quad F^{(32)}_{1234} = F^{(32)}_{3214},\\
&F^{(33)}_{1234} = F^{(33)}_{3214}\,, \quad F^{(34)}_{1234} = F^{(34)}_{3214}\,, \quad F^{(35)}_{1234} = F^{(35)}_{3412}\,,\\
&F^{(36)}_{1234} = F^{(36)}_{4321} = F^{(36)}_{3412}\,, \quad F^{(37)}_{123} = F^{(37)}_{213} = F^{(37)}_{231}\,. \qquad (6.11)
\end{aligned}
$$

We have indicated only the generators of the symmetry group (e.g. for $F^{(3)}$ it follows that this function is completely symmetric under permutations). As discussed before, only after imposing the symmetries can one expect the coefficient functions to be unique for a given functional. A subtlety that did not appear in the two or four derivative cases is that one has to take into account not only true symmetries but also *quasi-symmetries*. For instance,

$$
\begin{aligned}
&\left\langle F^{(31)}_{123} T_{31} \right\rangle = \left\langle F^{(31)}_{123} X_{\alpha\beta} Z_{\alpha\gamma} Z_{\beta\gamma} \right\rangle\\
&= \left\langle F^{(31)}_{432} Z_{\beta\gamma} Z_{\alpha\gamma} X_{\alpha\beta} \right\rangle\\
&= \left\langle F^{(31)}_{213} X_{\alpha\beta} Z_{\beta\gamma} Z_{\alpha\gamma} \right\rangle = \left\langle F^{(31)}_{213} X_{\beta\alpha} Z_{\alpha\gamma} Z_{\beta\gamma} \right\rangle\\
&= \left\langle F^{(31)}_{213} (X_{\alpha\beta} Z_{\alpha\gamma} Z_{\beta\gamma} + [Z_{\beta\alpha}, X] Z_{\alpha\gamma} Z_{\beta\gamma}) \right\rangle\\
&= \left\langle F^{(31)}_{213} X_{\alpha\beta} Z_{\alpha\gamma} Z_{\beta\gamma} + (X_1 - X_2) F^{(31)}_{213} Z_{\alpha\beta} Z_{\alpha\gamma} Z_{\beta\gamma} \right\rangle\\
&= \left\langle F^{(31)}_{213} T_{31} + (X_1 - X_2) F^{(31)}_{213} T_{37} \right\rangle\,, \qquad (6.12)
\end{aligned}
$$

therefore the antisymmetric component of $F^{(31)}_{123}$ under transposition of 12 can always be traded by a contribution to T_{37} and one can require $F^{(31)}_{123}$ to be symmetric.

To verify that the 37 structures are necessary we have used the following device. We consider a generic expression F of the type (6.1) with unspecified coefficient functions $F^{(i)}$. Then F is expanded in terms of *bare structures*, namely, structures formed with operators D_μ, as in the first equality of (6.6). There are five such bare structures,

$$
\begin{aligned}
&D_\alpha D_\alpha D_\beta D_\beta D_\gamma D_\gamma\,, \quad D_\alpha D_\alpha D_\beta D_\gamma D_\beta D_\gamma\,,\\
&D_\alpha D_\alpha D_\beta D_\gamma D_\gamma D_\beta\,, \quad D_\alpha D_\beta D_\alpha D_\gamma D_\beta D_\gamma\,,\\
&\text{and} \quad D_\alpha D_\beta D_\gamma D_\alpha D_\beta D_\gamma
\end{aligned}
$$

(modulo cyclic and mirror symmetries). The reason to do this is that an expression written in terms of bare structures is zero if and only if the corresponding coefficient functions vanish (after imposing the appropriate symmetry restrictions to those coefficients). That is, there are no identities (like Jacobi or integration by parts) in terms of bare structures, so two expressions are equal only if their (symmetrized) coefficient functions are equal. To see that a given structure T_i is necessary, i.e., that it cannot always be written in terms of the other structures, it is enough to

expand F as a power series of X in terms of bare structures and equate it to zero. If T_i were redundant, for any choice of $F^{(i)}$ there would be choices of the other coefficient functions so that the equation $F = 0$ would hold true at each order in the series expansion. It can be verified that this is not the case for any T_i when one considers the equations at order X^6.

In the six derivative case, we have not found a closed proof that the symmetrized coefficient functions associated to an expression are really unique. In principle there could exist non-trivial identities, that is, sets of non-vanishing functions $F^{(i)}$ producing a vanishing expression F. (If the $F^{(i)}$ were not symmetrized or the T_i were not all necessary, this would certainly be the case.) To investigate this issue, we have considered large classes of functions $F^{(i)}$ of the type encountered in B_3, i.e., obtained by linear combination of functions $I_{r_1,r_2,\ldots,r_n}$, with adjustable numerical coefficients. The corresponding expression has been expanded in terms of bare structures and equated to zero. No non-trivial identity has been found. Our conjecture is that the symmetrized coefficient functions corresponding to a given expression are unambiguous.

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Appendix

A Summary of the notation and conventions

In this appendix we collect several notational conventions used in the text.

$$K = D_\mu^2 + X\,, \quad D_\mu = \partial_\mu + V_\mu\,, \quad Z_{\mu\nu} := [D_\mu, D_\nu]\,. \tag{A.1}$$

$$\langle\ \rangle := \frac{1}{(4\pi\tau)^{d/2}} \int \mathrm{d}^d x\ \mathrm{tr}(\ )\,. \tag{A.2}$$

Units restoration:

$$a_n \to \tau^n a_n\,, \qquad B_n(X) \to \tau^n B_n(\tau X)\,. \tag{A.3}$$

Indices convention:

$$Y_{\mu I} = [D_\mu, Y_I]\,. \tag{A.4}$$

Symmetric functions:

$$I_{r_1,r_2,\ldots,r_n} = \prod_{\ell=1}^{n} \frac{1}{(r_\ell - 1)!} \left(\frac{\partial}{\partial X_\ell}\right)^{r_\ell - 1} \times \sum_{i=1}^{n} \mathrm{e}^{X_i} \prod_{j\neq i} \frac{1}{X_i - X_j}\,. \tag{A.5}$$

$$I_1 = \mathrm{e}^X\,,$$

$$I_{1,1} = \frac{\mathrm{e}^{X_1} - \mathrm{e}^{X_2}}{X_1 - X_2}\,, \tag{A.6}$$

$$I_{1,1,1} = \frac{\mathrm{e}^{X_1} - \mathrm{e}^{X_2}}{(X_1 - X_2)(X_2 - X_3)} - \frac{\mathrm{e}^{X_1} - \mathrm{e}^{X_3}}{(X_1 - X_3)(X_2 - X_3)}\,.$$

Mirror transformation:

$$AB \to B^{\mathrm{T}} A^{\mathrm{T}}\,, \quad X_{\mu_1\ldots\mu_n} \to X_{\mu_1\ldots\mu_n}\,, \quad Z_{\mu_1\ldots\mu_n} \to -Z_{\mu_1\ldots\mu_n}\,. \tag{A.7}$$

Mirror symmetry convention:

$$Y := \frac{1}{2}(Y + Y^{\mathrm{T}})\,. \tag{A.8}$$

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