Covariant derivative expansion of the heat kernel

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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.

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I. INTRODUCTION AND CONCLUSIONS

Ever since its introduction by Schwinger [1], the heat kernel of Laplace-type operators has become 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 \( \zeta \)-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, 13, 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, 18, 19, 20, 21, 22, 23, 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, 28]. 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, 33, 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 Section III 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 IV is devoted to explaining the technique of labeled operators [33, 34, 37, 38]. Such procedure allows 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 Section V the diagonal heat kernel coefficients, within the derivative expansion, are obtained to

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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 

Section gives the six derivative contribution. It is based on previous results for the effective action found in . 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 Section VI 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 . 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 , 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 , which only requires to replace the integral over coordinate 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.

## II. 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

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

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

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

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

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

where \( A_n(x) \) depends on \( \tau \) 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 \( \tau \), \( A_n \) has dimension \( 2n \).) Technically, the covariant derivative expansion can be defined by introducing a bookkeeping parameter \( \lambda \) by means of \( X(x) \to X(\lambda x) \) and \( V_\mu(x) \to \lambda V_\mu(\lambda x) \), and then expanding the functional.
$\langle \lambda^{-1} \rangle |e^{\tau K(\lambda)}| \lambda^{-1} \rangle$ in powers of $\lambda$. 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)

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

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

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

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

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

$$\text{Tr} e^K = \int d^d x \text{tr} \langle x|e^K|x \rangle. \quad (2.7)$$

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

$$\langle \rangle := \frac{1}{(4\pi)^{d/2}} \int d^d x \text{tr} ( ) \quad (2.8)$$

the standard and derivative expansions take the form

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

In $\text{Tr} e^K$ 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

$$\langle b_n \rangle = \langle a_n \rangle, \quad \langle B_n \rangle = \langle A_n \rangle. \quad (2.10)$$

In particular,

$$\text{Tr} e^K = \sum_{n=0}^{\infty} \langle B_n \rangle. \quad (2.11)$$

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 Section IV).

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)

$$\text{Tr} \log K = \int \frac{d^d x d^d k}{(2\pi)^d} \text{tr} \left( -\log N + \frac{k^2}{d} N^2 + \cdots \right), \quad (2.12)$$

1 Our notational conventions are summarized in Appendix A.
where
\[ N = (k^2 - X)^{-1}, \quad N_\mu = [D_\mu, N]. \] (2.13)

In what follows we will consistently use the convention\(^2\) \( Y_{\mu} = [D_\mu, Y_I] \) where \( Y_I \) is an object (such as \( N, X \) or \( Z \)) with an ordered set of Lorentz indices \( I \). So for instance\(^3\)
\[ X_{\mu\nu} = [D_\mu, [D_\nu, X]], \quad Z_{\mu\nu\lambda} = [D_\mu, [D_\nu, D_\lambda]]. \] (2.14)

The formula (2.12) holds modulo a counter term action which must be a local polynomial (in \( X, V_\mu \) and \( \partial_\mu \)) of degree at most \( d \). Such counter terms depend on the renormalization prescription chosen. The derivative expansion of the effective action can be written as
\[ \text{Tr} \log K = \int \frac{d^d x d^d k}{(2\pi)^d} \sum_{n=0}^{\infty} k^{2n} \frac{\Gamma(d/2)\text{tr}(F_n)}{\Gamma(n+d/2)}. \] (2.15)

Each \( F_n \) is gauge covariant, contains a number \( 2n \) of \( D_\mu \)'s and a number \( 2n \) of \( N \)'s, and has no explicit dependence on the space-time dimension \( d \). To four derivatives
\[ F_0 = -\log N, \quad F_1 = \frac{1}{2} N_\mu^2, \quad F_2 = N_\mu^2 N_\nu^2 - \frac{1}{2} (N_\mu N_\nu)^2 - (NN_\mu\mu)^2 - 2NZ_{\mu\nu}NN_\mu N_\nu - \frac{1}{2} (Z_{\mu\nu}N^2)^2. \] (2.16)

These terms were obtained in \(^4\). The six derivative term \( F_3 \) is given in (5.1). It was obtained in \(^3\) 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 Section V. 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:
\[ e^K = \int_{\Gamma} \frac{dz}{2\pi i} \frac{e^z}{z - K} = \int_{\Gamma} \frac{dz}{2\pi i} e^z \frac{d}{dz} \log(K - z) = -\int_{\Gamma} \frac{dz}{2\pi i} e^z \log(K - z). \] (2.17)

Here \( \Gamma \) 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 (2.16) to \( \text{Tr} \log(K - z) \), i.e., with the replacement \( X \to X - z \). The first thing to note is that the counter term 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 \( \text{Tr} \) in (2.17) and inserting (2.15), one finds that all non explicit dependence on \( k_\mu \) comes in the form \( X - k^2 - z \). Making the shift \( z \to z - k^2 \) removes all dependence on \( k_\mu \) in \( F_n \). (Such change of variables is justified at the level of asymptotic expansions we are considering.) Straightforward momentum integration gives then
\[ \text{Tr} e^K = -\sum_{n=0}^{\infty} \int_{\Gamma} \frac{dz}{2\pi i} e^z \langle F_n \rangle, \] (2.18)
that is,
\[ B_n = -\int_{\Gamma} \frac{dz}{2\pi i} e^z F_n \] (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
\[ N = (z - X)^{-1}. \] (2.20)

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\(^2\) Here and elsewhere in this work \( Y \)' stands for a generic matrix-valued function.

\(^3\) Note that in \(^3\) the convention \( Y_{\mu} = [D_\mu, Y_I] \) is used instead. Also \( F_{\mu\nu} \) there corresponds to \( iZ_{\mu\nu} \) here.

\(^4\) Note that the sign of the fourth term of \( F_2 \) is incorrect in \(^3\).
The integration over \( z \) is easily done for the zeroth order term (undoing the steps in \((2.17)\))

\[
B_0 = \int \frac{dz}{2\pi i} e^z \log N = \int \frac{dz}{2\pi i} e^z = e^x.
\]

(2.21)

For \( B_1 \), we first expand the covariant derivative using the identity

\[
N_\mu = N X_\mu N
\]

(2.22)

so that \( z \) appears only in \( N \) outside covariant derivatives

\[
F_1 = \frac{1}{2} N^2 X_\mu N^2 X_\mu
\]

(2.23)

(operators at position 3 can be moved 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 \( X_\mu \) in \((2.23)\) there are three positions, namely, the position 1 at the left of the first (leftmost) \( X_\mu \), the position 2, in between the two \( X_\mu \) and the position 3, after the second \( X_\mu \). (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 \( X_\mu \) 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

\[
F_1 = \frac{1}{2} N^2 N_2^2 X_\mu X_\mu = \frac{1}{2} \frac{1}{(z - X_1)^2} \frac{1}{(z - X_2)^2} X_\mu^2.
\]

(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 \( X_\mu \)). 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 Section III 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

\[
\langle B_1 \rangle = \langle f(X_1, X_2) X_\mu^2 \rangle
\]

(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

\[
f(x, y) = -\frac{1}{2} \int_{\Gamma} \frac{dz}{2\pi i} e^z \frac{1}{(z - x)^2} \frac{1}{(z - y)^2} = \frac{e^x - e^y}{(x - y)^3} - \frac{1}{2} \frac{e^x + e^y}{(x - y)^2}.
\]

(2.26)

(By definition \( \Gamma \) 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)

\[
\langle B_1 \rangle = \sum \left( \left( \frac{-1}{12} - \frac{1}{24} (X_1 + X_2) - \frac{1}{80} (X_1^2 + X_2^2) - \frac{1}{60} X_1 X_2 + \cdots \right) X_\mu^2 \right)
\]

\[
= \sum \left( \frac{-1}{12} X_\mu^2 - \frac{1}{12} X X_\mu - \frac{1}{24} X^2 + \frac{1}{40} X^2 + \frac{1}{60} X X_\mu + \cdots \right).
\]

(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

\[
F_2 = (N^2 X_\mu N^2 X_\mu)^2 - \frac{1}{2} (N^2 X_\mu N^2 X_\nu)^2 - 4 (N^3 X_\mu N X_\mu)^2 - (N^3 X_\mu X_\mu)^2
\]

\[
= -4N^3 X_\mu N X_\mu N X_\mu - 2N^2 X_\mu N X_\mu N X_\mu - \frac{1}{2} (N^2 Z_\mu)^2
\]

\[
= N_1^2 N_2^2 N_3^2 N_4^2 (X_\mu X_\nu)^2 - \frac{1}{2} N_1^2 N_2^2 N_3^2 N_4^2 (X_\mu X_\nu)^2 - 4N_1^3 N_2^3 N_3^3 N_4 (X_\mu X_\nu)^2 - N_1^3 N_2^3 X_\mu X_\mu
\]

\[
= -4N_1^3 N_2^3 N_3^3 X_\mu X_\nu - 2N_1^2 N_2^2 N_3^3 X_\mu X_\nu Z_\mu - \frac{1}{2} N_1^2 N_2^2 Z_\mu.
\]

(2.28)
The integrals over \( z \) involved in the computation of the \( B_n \) are of the form

\[
I_{r_1, r_2, \ldots, r_n}(X_1, X_2, \ldots, X_n) := \int \frac{dz}{2\pi i} e^z N_{r_1}^1 N_{r_2}^2 \cdots N_{r_n}^n.
\]  

They can be computed from the basic integrals

\[
I_n^0(X_1, X_2, \ldots, X_n) := \int \frac{dz}{2\pi i} e^z N_1 N_2 \cdots N_n = \sum_{i=1}^n e^{X_i} \prod_{j \neq i} \frac{1}{X_i - X_j}
\]  

Using

\[
I_{r_1, r_2, \ldots, r_n}(X_1, X_2, \ldots, X_n) = \prod_{i=1}^n \frac{1}{(r_i - 1)!} \left( \frac{\partial}{\partial X_i} \right)^{r_i-1} I_n^0(X_1, X_2, \ldots, X_n).
\]  

(Alternatively, \( I_{r_1, r_2, \ldots, r_n}(X_1, X_2, \ldots, X_n) \) can be obtained from \( I_n^0 \) 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

\[
I_n^0(X_1) = e^{X_1},
\]

\[
I_{n+1}^0(X_1, \ldots, X_{n+1}) = \frac{I_{n}^0(X_1, \ldots, X_{n+1-1}, X_{n+1-1}) - I_{n}^0(X_1, \ldots, X_{n+1-1}, X_{n+1})}{X_{n+1-1} - X_{n+1}}.
\]  

We will use the short-hand notation

\[
I_{r_1, r_2, \ldots, r_n} := I_{r_1, r_2, \ldots, r_n}(X_1, X_2, \ldots, X_n).
\]  

With this notation the lowest terms in the derivative expansion are

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

Expanding in powers of \( X \) one obtains for \( B_2 \)

\[
\langle B_2 \rangle = \left( \frac{1}{12} Z_{\mu\nu}^2 + \frac{1}{12} X Z_{\mu\nu}^2 + \frac{1}{40} X^2 Z_{\mu\nu}^2 + \frac{1}{60} (X Z_{\mu\nu})^2 + \frac{1}{60} X_{\mu\nu} Z_{\mu\nu} + \frac{1}{120} X_{\mu\nu}^2 + \frac{1}{180} X^3 Z_{\mu\nu}^2 + \frac{1}{120} X^2 Z_{\mu\nu} Z_{\mu\nu} + \frac{1}{180} (X X_{\mu\nu} Z_{\mu\nu} + X_{\mu\nu} X_{\mu\nu} Z_{\mu\nu} + X_{\mu\nu} X_{\mu\nu} Z_{\mu\nu} + \frac{1}{180} X_{\mu\nu}^2 X_{\mu\nu} + \cdots \right)
\]  

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

The expressions \([2, 3]\), 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

\[
\langle f(X_1, X_2, X_3, X_4) X_\mu^2 X_\mu^2 \rangle = \langle f(X_3, X_4, X_1, X_2) X_\mu^2 X_\mu^2 \rangle
\]  

(2.36)
shows that one can always choose the coefficient function of $(X^2_\mu)^2$ to be invariant under the cyclic permutation $(X_1, X_2, X_3, X_4) \rightarrow (X_3, X_4, X_1, X_2)$ and this symmetry is explicit in $(B_2)$ given in 2.34 using the permutation symmetry properties of the functions $I_{r_1,r_2,...,r_n}$.

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
\[(AB)^T = B^T A^T, \quad D^T_\mu = D_\mu, \quad X^T = X. \tag{2.37}\]

They imply $[D_\mu, Y]^T = -[D_\mu, Y^T]$ and thus
\[X^T_{\mu_1...\mu_n} = (-1)^n X_{\mu_1...\mu_n}, \quad Z^T_{\mu_1...\mu_n} = (-1)^{n-1} Z_{\mu_1...\mu_n}. \tag{2.38}\]

In practice, because the total number of Lorentz indices is always even, an equivalent rule is to pick up a minus sign for each $Z_{\mu_1...\mu_n}$ 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.
\[
\langle (X_1, X_2, X_3)X^2_\mu X_{\nu}\rangle^T = \langle (X_1, X_3, X_2)X_{\nu}X^2_\mu\rangle = \langle (X_3, X_2, X_1)X^2_\mu X_{\nu}\rangle \tag{2.39}
\]
shows that the coefficient function of $X^2_\mu X_{\nu}$ (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.

### III. 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.\(^5\)
\[f(A_1, B_2, C_3, \ldots)XY \cdots \tag{3.1}\]

$X, Y, \text{etc.}$ are the fixed operators in this case, $A$ is to be inserted before (to the left of) $X$ (position 1), $B$ between $X$ 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.
\[f(x_1, x_2, x_3, \ldots) = \sum_{n_1, n_2, n_3, \ldots} c_{n_1, n_2, n_3, \ldots} x_1^{n_1} x_2^{n_2} x_3^{n_3} \cdots,
\]
\[f(A_1, B_2, C_3, \ldots)XY \cdots := \sum_{n_1, n_2, n_3, \ldots} c_{n_1, n_2, n_3, \ldots} A^{n_1} X B^{n_2} Y C^{n_3} \cdots. \tag{3.2}\]

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 being $\langle n, A\rangle$, the corresponding dual basis,
\[\langle n, A|f(A_1, B_2, C_3)XY|r, C\rangle = \sum_{m} f(a_n, b_m, c_r) \langle n, A|m, B\rangle \langle m, B|Y|r, C\rangle. \tag{3.3}\]

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. $A_1 B_2 = B_2 A_1$, 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
\[e^{[A, \ ]}X = e^{A}Xe^{-A} \tag{3.4}\]
becomes trivial using labeled operators
\[e^{[A, \ ]}X = e^{A_1 - A_2}X = e^{A_1}e^{-A_2}X = e^{A}Xe^{-A}. \tag{3.5}\]

\(^5\) The symbols $A, B, X, \text{etc.}$, are generic and do not refer to those of the heat kernel throughout this Section.
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

\[
e^{A+B} = e^{A} + \int_0^1 ds e^{sA}Be^{(1-s)A} + O(B^2).
\]

(3.6)

Using labeled operators one can go further and obtain

\[
e^{A+B} = e^{A} + \int_0^1 ds e^{sA_1} + (1-s)A_2B + O(B^2) = e^{A} + \frac{e^{A_1} - e^{A_2}}{A_1 - A_2}B + O(B^2)
\]

(3.7)

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

\[
f(A + B) = f(A) + \frac{f(A_1) - f(A_2)}{A_1 - A_2}B + O(B^2).
\]

(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 \(\delta A\) of the operator \(A\) (the function \(f\) being unchanged)

\[
\delta (f(A)) = \nabla f(A_1, A_2)\delta A
\]

(3.9)

where the operation \(\nabla\) is defined by

\[
\nabla f(x_1, x_2) := \frac{f(x_1) - f(x_2)}{x_1 - x_2}.
\]

(3.10)

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

\[
\partial_\mu f(A) = \nabla f(A_1, A_2)\partial_\mu A
\]

(3.11)

or a commutator, \(\delta = [X, ]\),

\[
[X, f(A)] = \nabla f(A_1, A_2)[X, A]
\]

(3.12)

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

The operator \(\nabla\) generalizes the ordinary derivative to the non Abelian case. Of course, when \(A\) and \(\delta A\) commute the right-hand side of (3.12) becomes \(f'(A)\delta A\) (applying L’Hôpital rule). It is straightforward to verify that the operator \(\nabla\) satisfies a Leibniz rule

\[
\nabla (fg)(x_1, x_2) = \nabla f(x_1, x_2)g(x_2) + f(x_1)\nabla g(x_1, x_2),
\]

(3.13)

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

\[
\nabla (f \circ g)(x_1, x_2) = \nabla f(g(x_1), g(x_2))\nabla g(x_1, x_2)
\]

(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.

\[
\delta(f(A_1, B_2)X) = \nabla_1 f(A_1, A_2, B_3)\delta A X + \nabla_2 f(A_1, B_2, B_3)X \delta B + f(A_1, B_2)\delta X,
\]

(3.15)

\(^6\) 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 \(A\).
where \( \nabla_\ell \) indicates that it acts on the \( \ell \)-th argument of \( f \).

It is also convenient to define a \( \nabla \) 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

\[
\nabla := \sum_k \nabla_k
\]

(\( \nabla_k \) acting on the \( k \)-th argument of the function) and so

\[
\nabla f(x_1, \ldots, x_{n+1}) = \sum_{k=1}^n \frac{f(x_1, \ldots, \widehat{x_{k+1}}, \ldots, x_{n+1}) - f(x_1, \ldots, x_k, \ldots, x_{n+1})}{x_k - x_{k+1}},
\]

where \( \widehat{x_\ell} \) indicates that the \( \ell \)-th argument is missing. The definition is such that

\[
\delta \left( f(A_1, \ldots, A_n)(\delta A)^{n-1} \right) = \nabla f(A_1, A_2, \ldots, A_{n+1})(\delta A)^n
\]

(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

\[
f(A + B) = e^{B\nabla A} f(A)
\]

(3.19)

(\( \nabla_A \) emphasizes that \( \nabla \) acts on the \( A \)-dependence of the expression). That is

\[
f(A + B) = f(A) + \nabla f(A_1, A_2)B + \frac{1}{2!} \nabla^2 f(A_1, A_2, A_3)B^2 + \cdots
\]

\[
= f(A) + \frac{f(A_1) - f(A_2)}{A_1 - A_2}B + \left( \frac{f(A_1)}{(A_2 - A_1)(A_3 - A_1)} + \frac{f(A_2)}{(A_1 - A_2)(A_3 - A_2)} + \frac{f(A_3)}{(A_1 - A_3)(A_2 - A_3)} \right) B^2 + \cdots.
\]

(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 \( f(A_1, A_2, \ldots) \) 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

\[
\frac{1}{A_1 - A_2}B
\]

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

**IV. 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 (4)

\[
\delta_X \text{Tr} e^{D^2_n + X} = \text{Tr} \left( e^{D^2_n + X} \delta X \right)
\]

(4.1)

where \( \delta_X \) is a first order variation with respect to \( X \). That is

\[
\langle x | e^K | x \rangle = \frac{\delta \text{Tr} e^K}{\delta X(x)}.
\]

(4.2)

For the Seeley-DeWitt coefficients this implies

\[
a_n(x) = (4\pi)^{d/2} \frac{\delta(b_{n+1})}{\delta X(x)}.
\]

(4.3)
whereas for the derivative expansion coefficients gives

\[ A_n(x) = (4\pi)^{d/2} \frac{\delta \langle B_n \rangle}{\delta X(x)}. \]  

(4.4)

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

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

(4.5)

It can be shown that this consistency condition is satisfied by our expressions \[ \frac{\delta \langle B_n \rangle}{\delta X(x)} \]. This only requires the property

\[ \delta X N = N \delta X N. \]  

(4.6)

(this relation codifies the heat kernel property \( e^K \rightarrow e^{\alpha K} \) under the shift \( X \rightarrow X + \alpha, \alpha \) 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 \( \exp(X + f(D^2_n)) \).

Using the results in Section \[ \text{III} \] 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 \[ (4.5) \]. 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

\[ \delta_X N = N \delta X N. \]  

(4.7)

We illustrate the method with \( A_1 \):

\[ \delta_X \langle F_1 \rangle = \delta_X \left( \frac{1}{2} N^2 X_\mu X^2 \mu \right) = \langle N \delta X N^2 X_\mu + N^2 \delta X N X_\mu \rangle \]

\[ = \langle (N^2 X_\mu X_\nu N + N X_\mu X_\nu N^2 - (N^2 X_\mu N^2) \mu) \delta X \rangle \]

\[ = \langle (2N^2 X_\mu X_\nu - N^2 X_\mu N^2) \delta X \rangle. \]

i.e.

\[ \frac{\delta \langle F_1 \rangle}{\delta X} = \frac{1}{(4\pi)^{d/2}} \left( 2N^2 X_\mu X_\nu + N^2 X_\mu \right). \]

(4.8)

(4.9)

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

\[ A_0 = I_1, \]

\[ A_1 = 2I_2,1,2X^2_\mu + I_2,2X_{\mu \nu}, \]

\[ A_2 = 2I_2,1,2Z_{\mu \nu}Z_{\mu \nu} \]

\[ + (4I_{2,2,2} - 8I_{3,0,3} + 8I_{2,1,1,3}) Z_{\mu \nu}X_\nu \]

\[ + (4I_{2,1,2} - 16I_{3,0,1,1,3}) X_\mu Z_{\mu \nu}X_\nu \]

\[ + (32I_{3,0,1,1,3} - 16I_{2,1,1,1,3} - 8I_{2,2,1,2} + 16I_{3,0,2,2}) Z_{\mu \nu}X_\mu X_\nu \]

\[ + (2I_{3,3} + 4I_{2,2,3}) X_{\mu \nu}X_{\mu \nu} \]

\[ + 8I_{3,3}X_{\mu \nu}X_{\mu \nu} \]

\[ + (16I_{3,1,3} + 8I_{3,2,2}) X_{\mu \nu}X_\mu \]

\[ + (4I_{2,2,2} + 16I_{3,1,1,3} + 16I_{2,2,1,3}) X_\mu X_{\mu \nu}X_\nu \]

\[ + (2I_{2,2,2} + 8I_{3,1,1,3} + 8I_{2,2,1,3}) X_\mu X_{\nu \mu}X_\nu \]

\[ + (4I_{2,2,2} + 16I_{3,1,1,3} + 8I_{2,2,1,1,3} + 8I_{3,1,2,2} + 8I_{2,2,2,1,2}) X_{\mu \nu}X_\nu X_\nu \]

\[ + (32I_{3,1,1,1,3} + 16I_{3,1,1,2,2}) X_\mu X_{\mu \nu}X_\nu \]

\[ + (4I_{2,2,2} + 16I_{3,1,1,1,3} + 16I_{2,2,2,1,3}) X_\mu X_{\mu \nu}X_\nu \]

\[ + (4I_{2,2,2,2} + 16I_{3,1,1,1,3} + 16I_{2,2,2,1,3}) X_{\mu \nu}X_{\mu}X_\nu \]

\[ + (4I_{2,2,1,2,2} + 16I_{3,1,1,1,3} + 16I_{2,2,1,1,1,3}) X_{\mu}X_{\mu}X_{\nu} \]

\[ + (2I_{2,2,1,2,2} + 16I_{3,1,1,1,1,3} + 16I_{2,2,1,1,1,3}) X_{\mu}X_{\nu}X_\mu. \]  

(4.10)
\( A_1 \) is a direct transcription of (1.8). 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,

\[
4I_{2,2,3} X_{\mu \nu} X_{\mu \nu} := (2I_{2,2,3} + 2I_{3,0,2,2}) X_{\mu \nu} X_{\mu \nu}, \\
16I_{3,0,2,2} Z_{\mu \nu} X_{\mu} X_{\nu} := 8I_{3,0,2,2} Z_{\mu \nu} X_{\mu} X_{\nu} + 8I_{2,2,0,3} X_{\mu} X_{\nu} Z_{\mu \nu} .
\] (4.11)

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

\[
Y_{\mu \nu} = Y_{\nu \mu} + [Z_{\mu \nu}, Y]
\] (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.

V. SIX DERIVATIVE TERMS, \( B_3 \)

The term \( F_3 \) in the expansion (2.16) has been computed in (3.2):

\[
F_3 = \frac{20}{3} N_a N_b N_c N_d N_e N_f N_g - N_a N_b N_c N_d N_e N_f N_g + \frac{2}{3} N_a N_b N_c N_d N_e N_f N_g + 2 N_a N_b N_c N_d N_e N_f N_g
\]

\[
-4 N_a N_b N_c N_d N_e N_f N_g - 16 N_a N_b N_c N_d N_e N_f N_g + 6 N_a N_b N_c N_d N_e N_f N_g
\]

\[
-16 N_a N_b N_c N_d N_e N_f N_g - 8 N_a N_b N_c N_d N_e N_f N_g - 16 N_a N_b N_c N_d N_e N_f N_g
\]

\[
+8 N_a N_b N_c N_d N_e N_f N_g + 10 N_a N_b N_c N_d N_e N_f N_g - 4 N_a N_b N_c N_d N_e N_f N_g
\]

\[
\frac{8}{3} N_a N_b N_c N_d N_e N_f N_g + 12 N_a N_b N_c N_d N_e N_f N_g + 3 N_a N_b N_c N_d N_e N_f N_g
\]

\[
-8 N_a N_b N_c N_d N_e N_f N_g - 4 N_a N_b N_c N_d N_e N_f N_g - 8 N_a N_b N_c N_d N_e N_f N_g - 8 N_a N_b N_c N_d N_e N_f N_g
\]

\[
-16 N_a N_b N_c N_d N_e N_f N_g - 8 N_a N_b N_c N_d N_e N_f N_g - 16 N_a N_b N_c N_d N_e N_f N_g
\]

\[
-16 N_a N_b N_c N_d N_e N_f N_g - 8 N_a N_b N_c N_d N_e N_f N_g
\]

\[
\frac{4}{3} N_a N_b N_c N_d N_e N_f N_g
\] (5.1)

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 (3.2). In order to obtain the heat kernel coefficient \( B_3 \) from \( F_3 \) we use the procedure of Section 11 as in e.g. (2.28). This yields

\[
(B_3) = \left\{ -3 I_{414} X_{\alpha \beta \gamma} X_{\alpha \gamma} - 24 I_{414} X_{\alpha \beta \gamma} X_{\alpha \gamma} + (-12 I_{414} - 12 I_{414}) X_{\alpha \beta \gamma} X_{\alpha \gamma}
\]

\[
+ \frac{8}{3} I_{3123} X_{\alpha \beta \gamma} X_{\alpha \gamma} + (-24 I_{414} - 24 I_{414}) X_{\alpha \beta \gamma} X_{\alpha \gamma} - 12 I_{4114} X_{\alpha \beta \gamma} X_{\alpha \gamma}
\]

\[
+ (-12 I_{3124} - 6 I_{4114} - 6 I_{4221} + 16 I_{2323} + 4 I_{2323} + 16 I_{3133}) X_{\alpha \beta \gamma} X_{\alpha \gamma}
\]

\[
+ (-24 I_{4114} - 24 I_{2314}) X_{\alpha \beta \gamma} X_{\alpha \gamma} + 8 I_{3122} X_{\alpha \beta \gamma} X_{\alpha \gamma} - 8 I_{3222} X_{\alpha \beta \gamma} X_{\alpha \gamma}
\]

\[
-24 I_{4141} X_{\alpha \beta \gamma} X_{\alpha \gamma} + (-24 I_{4141} - 24 I_{2314} + 16 I_{3122}) X_{\alpha \beta \gamma} X_{\alpha \gamma} + 8 I_{3222} X_{\alpha \beta \gamma} X_{\alpha \gamma}
\]

\[
-24 I_{4141} X_{\alpha \beta \gamma} X_{\alpha \gamma} + (-24 I_{4141} - 12 I_{4223} - 10 I_{2323} + 8 I_{2323}) X_{\alpha \beta \gamma} X_{\alpha \gamma}
\]

\[
+ (-24 I_{4141} - 24 I_{4141} + 24 I_{2221}) + 32 I_{2211} - 24 I_{3123} + 32 I_{3123} + 32 I_{3133}
\]

\[
+ 16 I_{3223} + 32 I_{3123} + 32 I_{3133} + 32 I_{3133} + 32 I_{3133}
\]

\[
+ (-84 I_{4114} - 48 I_{4112}) X_{\alpha \beta \gamma} X_{\alpha \gamma} + 16 I_{3212} X_{\alpha \beta \gamma} X_{\alpha \gamma}
\]

\[
+ (-16 I_{3212} - 16 I_{2223} + 32 I_{3132} - 48 I_{4114} + 48 I_{4123}) X_{\alpha \beta \gamma} X_{\alpha \gamma}
\]

\[
+ (-24 I_{4132} - 24 I_{4114} - 16 I_{2133} - 40 I_{2133} - 24 I_{2141} - 16 I_{3122}) X_{\alpha \beta \gamma} X_{\alpha \gamma}
\]

\[
+ (-24 I_{4132} - 24 I_{4114} - 16 I_{2133} - 40 I_{2133} - 24 I_{2141} - 16 I_{3122}) X_{\alpha \beta \gamma} X_{\alpha \gamma}
\]

\[
+ (-24 I_{3123} - 24 I_{4114} - 16 I_{2133} - 40 I_{2133} - 24 I_{2141} - 16 I_{3122}) X_{\alpha \beta \gamma} X_{\alpha \gamma}
\]

\[
+ (-24 I_{3123} - 24 I_{4114} - 16 I_{2133} - 40 I_{2133} - 24 I_{2141} - 16 I_{3122}) X_{\alpha \beta \gamma} X_{\alpha \gamma}
\]
done in \[39\] for a smaller number of structures, but this is unlikely. The price to pay for a smaller number of structures is to increase that problem in this Section.

Instead of finding shortest expressions, it is also of interest to find a standard basis \[40, 41\] of structures. We discuss as explained at length in \[39\], the expression of \( F \) could be written using a standard basis of structures with 37 elements. (Conceivably, a concrete functional such as \( F \)’s. Similarly, \( B \) can be written using a combination of functions \( I_1, r_2, \ldots, r_n \). 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 \[41\] 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.

### VI. 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 \( D_\mu \) 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:

\[
(F) = \sum_{i=1}^{N} \left< F^{(i)}(X_1, X_2, \ldots)T_i \right>
\]  

(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 (6.3) suggest that the following are standard basis for gauge invariant functionals with cyclic and mirror symmetry: For zero derivatives,

\[
T_1 = 1.
\]  

(6.2)

For functionals with two derivatives

\[
T_1 = X^2_\mu,
\]  

(6.3)

and for four covariant derivatives,

\[
T_1 = (X^2_\mu)^2, \quad T_2 = (X_\mu X_\nu)^2, \quad T_3 = X^2_{\mu\nu}, \quad T_4 = X^2_\mu X_\nu, \quad T_5 = X_\mu X_\nu Z_{\mu\nu}, \quad T_6 = Z^2_{\mu\nu}.
\]  

(6.4)

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

\[
\langle f(X) X_{\mu\nu} \rangle = \langle -[D_\mu, f(X)] X_\mu \rangle = \langle -\nabla f(X_1, X_2) X^2_\mu \rangle = \langle F^{(1)}(X_1, X_2) T_1 \rangle.
\]  

(6.5)

As we have noted at the end of Section III, 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 attended 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

\[
\langle f(X_1, X_2) X^2_\mu \rangle = \langle f(X_1, X_3)(X_1 - 2X_2 + X_3)(X_3 - 2X_4 + X_1)D_\mu D_\mu D_\nu D_\nu \rangle
\]

\[
= \langle f(X_1, X_3) \frac{(X_1 - 2X_2 + X_3)(X_3 - 2X_4 + X_1)}{(X_2 - X_1)(X_3 - X_2)(X_4 - X_3)(X_1 - X_4)} X_\mu X_\mu X_\nu X_\nu T_1 \rangle
\]

\[
= \langle F^{(1)}(X_1, X_2, X_3, X_4) T_1 \rangle.
\]  

(6.6)

Such 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 \( X^2_\mu \), 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 \( \langle f(X_1, X_2) X^2_\mu \rangle \) 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 \( \langle F^{(1)}(X_1, X_2) X^2_\mu \rangle \) 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

\[
F^{(1)}_{1234} = F^{(1)}_{1432} = F^{(1)}_{1342} = F^{(1)}_{3412},
\]

\[
F^{(2)}_{1234} = F^{(2)}_{1432} = F^{(2)}_{2143} = F^{(2)}_{2341} = F^{(2)}_{3214} = F^{(2)}_{3412} = F^{(2)}_{4123} = F^{(2)}_{4321},
\]

\[
F^{(3)}_{12} = F^{(3)}_{21},
\]

\[
F^{(4)}_{123} = F^{(4)}_{321},
\]

\[
F^{(5)}_{123} = F^{(5)}_{321},
\]

\[
F^{(6)}_{12} = F^{(6)}_{21},
\]  

(6.7)
where we use a shorthand notation e.g. $F_{1432}^{(2)} = F^{(2)}(X_1, X_4, X_3, X_2)$. For instance

$$
\left\langle F_{123}^{(5)} X_\mu X_\nu Z_{\mu\nu} \right\rangle = - \left\langle F_{4321}^{(5)} Z_{\mu\nu} X_\mu X_\nu \right\rangle = - \left\langle F_{321}^{(5)} X_\mu Z_{\mu\nu} \right\rangle = \left\langle F_{321}^{(5)} X_\mu X_\nu Z_{\mu\nu} \right\rangle
$$

(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

$$
T_1 = X_\alpha X_\beta, T_2 = X_\alpha X_\beta X_\gamma, T_3 = X_\alpha X_\beta X_\gamma X_\beta, T_4 = X_\alpha X_\beta X_\gamma X_\beta X_\gamma, T_5 = X_\alpha X_\beta X_\gamma X_\alpha X_\beta X_\gamma, T_6 = X_\alpha X_\beta X_\gamma X_\alpha X_\beta X_\gamma X_\beta, T_7 = X_\alpha X_\beta X_\gamma X_\alpha X_\beta X_\gamma X_\beta X_\gamma, T_8 = X_\alpha X_\beta X_\gamma X_\alpha X_\beta X_\gamma X_\beta X_\gamma X_\alpha
$$

(6.9)

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 $\alpha$ in $X_\alpha X_\beta X_\gamma X_\beta$. Next, one can use the Jacobi identity (1.12) to choose the order of the covariant derivatives within each factor, for instance, if $X_\alpha X_\beta X_\gamma$ is retained, $X_\alpha X_\beta X_\gamma X_\beta$ becomes redundant. For the same reason all structures of the type $(\cdots Y_{\cdots \alpha \beta \gamma} \cdots Z_{\cdots \alpha \beta})$ are also redundant. Finally, $X_\alpha X_\beta X_\gamma Z_{\alpha \beta \gamma}$ can be reduced to $T_{21}$ using the Bianchi identity

$$
Z_{\alpha \beta \gamma} = Z_{\beta \alpha \gamma} + Z_{\gamma \alpha \beta}.
$$

(6.10)

This produces the set of structures in (5.3).

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

$$
F^{(1)}_{12} = F^{(1)}_{21}, \quad F^{(3)}_{123} = F^{(3)}_{123}, \quad F^{(4)}_{1234} = F^{(4)}_{1234}, \quad F^{(5)}_{12345} = F^{(5)}_{12345},
$$

$$
\begin{align*}
F^{(6)}_{123456} &= F^{(6)}_{123456}, \\
F^{(7)}_{1234567} &= F^{(7)}_{1234567}, \\
F^{(8)}_{12345678} &= F^{(8)}_{12345678}, \\
F^{(9)}_{123456789} &= F^{(9)}_{123456789}.
\end{align*}
$$

(6.11)

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,

$$
\left\langle F_{123}^{(31)} T_{31} \right\rangle = \left\langle F_{123}^{(31)} X_\alpha Z_{\alpha \gamma} Z_{\beta \gamma} \right\rangle = \left\langle F_{123}^{(31)} Z_{\beta \gamma} Z_{\alpha \gamma} X_\alpha \right\rangle = \left\langle F_{213}^{(31)} X_\alpha Z_{\alpha \beta} Z_{\beta \gamma} Z_{\alpha \gamma} \right\rangle
$$


\[ F^{(31)}_{213} X_{\beta\alpha} Z_{\alpha\gamma} Z_{\beta\gamma} = \left( F^{(31)}_{213} (X_{\alpha\beta} Z_{\alpha\gamma} Z_{\beta\gamma} + |Z_{\beta\alpha}, X| Z_{\alpha\gamma} Z_{\beta\gamma}) \right) \]
\[ = \left( F^{(31)}_{213} X_{\alpha\beta} Z_{\alpha\gamma} Z_{\beta\gamma} + (X_1 - X_2) F^{(31)}_{213} Z_{\alpha\beta} Z_{\alpha\gamma} Z_{\beta\gamma} \right) \]
\[ = \left( F^{(31)}_{213} T_{31} + (X_1 - X_2) F^{(31)}_{213} T_{37} \right), \tag{6.12} \]

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 (6.11) with unspecified coefficient functions \( F^{(i)} \). Then \( F \) is expanded in terms of bare structures, namely, structures formed with operators \( D_\mu \), as in the first equality of (6.10). There are five such bare structures, \( D_\alpha D_\alpha D_\beta D_\beta D_\gamma D_\gamma, D_\alpha D_\alpha D_\beta D_\gamma D_\beta D_\gamma, D_\alpha D_\beta D_\alpha D_\alpha D_\beta D_\gamma, D_\alpha D_\beta D_\alpha D_\beta D_\alpha D_\gamma \) and \( D_\alpha D_\beta D_\beta D_\gamma D_\alpha D_\beta D_\gamma \) (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 identities. 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 \( I_{r_1, r_2, ..., r_n} \), with adjustable numerical coefficients. The corresponding expression has been expanded in terms of bare structures and equated to zero. No nontrivial 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.

\[ K = D_\mu^2 + X, \quad D_\mu = \partial_\mu + V_\mu, \quad Z_{\mu\nu} := [D_\mu, D_\nu]. \tag{A1} \]

\[ \langle \, \rangle := \frac{1}{(4\pi r)^d/2} \int d^d x \, \text{tr} \left( \, \right). \tag{A2} \]

Units restoration:

\[ a_n \rightarrow \tau^n a_n, \quad B_n(X) \rightarrow \tau^n B_n(\tau X). \tag{A3} \]

Indices convention:

\[ Y_{\mu I} = [D_\mu, Y_I]. \tag{A4} \]

Symmetric functions:

\[ I_{r_1, r_2, ..., r_n} = \prod_{\ell=1}^{n} \frac{1}{(r_\ell - 1)!} \left( \frac{\partial}{\partial X_\ell} \right)^{r_\ell - 1} \sum_{i=1}^{n} \prod_{j \neq i}^{n} \frac{e^{X_i}}{X_i - X_j}. \tag{A5} \]
\[ I_1 = e^X, \]
\[ I_{1,1} = \frac{e^{X_1} - e^{X_2}}{X_1 - X_2}, \]
\[ I_{1,1,1} = \frac{e^{X_1} - e^{X_2}}{(X_1 - X_2)(X_2 - X_3)} - \frac{e^{X_1} - e^{X_3}}{(X_1 - X_3)(X_2 - X_3)}. \]  
\[ (A6) \]

Mirror transformation:
\[ AB \rightarrow B^T A^T, \quad X_{\mu_1 \ldots \mu_n} \rightarrow X_{\mu_1 \ldots \mu_n}, \quad Z_{\mu_1 \ldots \mu_n} \rightarrow -Z_{\mu_1 \ldots \mu_n}. \]  
\[ (A7) \]

Mirror symmetry convention:
\[ Y := \frac{1}{2} (Y + Y^T). \]  
\[ (A8) \]

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