HeatK: A Mathematica Program for Computing Heat Kernel Coefficients

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Heat kernel coefficients encode the short distance behavior of propagators in the presence of background fields, and are thus useful in quantum field theory. We present a Mathematica program for computing these coefficients and their derivatives, based on an algorithm by Avramidi [1].

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1. PROGRAM SUMMARY

Title of program: HeatK

Version number: 1.0

Available at: http://fermi.pha.jhu.edu/~booth/HeatK/

Programming Language: Mathematica 2.2 or higher

Platform: Any platform supporting Mathematica 2.2

Keywords: Heat kernel, HDMS coefficients, Effective Action

Nature of physical problem: Computation of heat kernel coefficients.

Method of solution: The non-recursive solution given by Avramidi \[1\]

Limitations: Degree of the heat kernel coefficient.

2. INTRODUCTION

Heat Kernel (also known as HDMS or Seeley-de Witt) coefficients have many applications in physics and mathematics (a comprehensive list can be found in a paper by Avramidi and Schwinnig \[2\]). Because of this interest, there is an extensive literature describing their computation and properties. Unfortunately for those who are primarily interested in using the coefficients as inputs to a calculation, there is not one comprehensive source for them, and moreover a number of different sign and normalization conventions are in use, making it difficult to combine sources. A further complication is that many applications require derivatives of the coefficients, of which only a few can be found in the literature. HeatK was created to resolve these problems and provide an environment which allows easy manipulation of the results.

3. THEORY

Consider a general manifold of dimension $d$ with metric $g_{\mu \nu}$, fields $\varphi^{(i)}$ and derivative $\nabla_\mu$ acting such that $[\nabla_\mu, \nabla_\nu] \varphi = F_{\mu \nu} \varphi$ and $[\nabla_\mu, \nabla_\nu] \varphi^\sigma = R^\sigma_{\tau \mu \nu} \varphi^\tau$. For a differential operator $H = -\Box + Q$, with $\Box = g_{\mu \nu} \nabla^\mu \nabla^\nu$ and $Q$ a matrix-valued potential, the heat kernel expansion is developed by considering the exponential $U(t) = \exp(-tH)$, which satisfies the equation

$$\frac{\partial U(t)}{\partial t} = -HU(t). \tag{1}$$

The kernel of the operator $U$ is then parameterized as

$$U(t|x, x') = \frac{1}{(4\pi t)^{d/2}} \Delta^{1/2} e^{-\sigma/2t} \sum_{k \geq 0} \frac{(-t)^k}{k!} a_k(x, x'), \tag{2}$$

where $a_k$ are the heat kernel coefficients, $\sigma(x, x')$ is half the square of the geodesic distance between the points $x$ and $x'$ and

$$\Delta(x, x') = g^{-1/2}(x) \det (-\nabla_\mu \nabla_\nu \sigma(x, x')) g^{-1/2}(x'). \tag{3}$$

is the Van Fleck-Morette determinant.

*We follow the conventions of Ref. \[1\] throughout.
The advantage of this machinery is that it allows us to take the familiar HDMS recursion relation:

\[ \sigma = [\sigma^\mu] = [\sigma^\mu] = 0, \]  

with \( f(x, x') \equiv \lim_{x \to x'} f(x, x') \).

It is also natural to define the tensor \( \eta^{\mu'}_{\nu'} = \nabla_\nu \sigma^{\mu'} \) and its inverse \( \gamma^\mu_{\nu} \). We can then define the parallel displacement operator \( P(x, x') \) as the solution to \( \sigma_\mu \nabla^\mu P = 0 \) with \( |P| = 1 \). When acting on vector indices, it is conventional to write \( g_{\mu\nu} \) instead of \( P_{\mu\nu} \). In what follows it is convenient to work with quantities bases at \( x' \), so we define \( \nabla^\mu = \gamma^\mu_{\nu} \nabla^\nu \) and the “gauge” field \( A_\mu = P^{-1} \nabla^\mu P \).

Introduce a functional basis

\[ |0\rangle \equiv 1, \]

\[ |n\rangle \equiv |\nu'_1 \ldots \nu'_n\rangle = \frac{(-1)^n}{n!} \sigma_{\nu'_1} \ldots \sigma_{\nu'_n}, \quad (n \geq 1), \]

its dual,

\[ \langle m| \equiv \langle \mu'_1 \ldots \mu'_m| = (-1)^m g_{\mu'_1} \ldots g_{\mu'_m} \nabla_{(\mu_1} \ldots \nabla_{\mu_m)} \delta(x, x'), \]

and the scalar product

\[ \langle m|n\rangle = \int d^n x \langle \mu'_1 \ldots \mu'_m| \nu'_1 \ldots \nu'_n\rangle, \]

so that

\[ \langle m|n\rangle = \delta_{mn} \delta^{\nu'_1 \ldots \nu'_n} = \delta_{mn} \delta^{\nu'_1} \ldots \delta^{\nu'_n}. \]

For a field \( \varphi \) we then have

\[ \langle m|\varphi\rangle = \left[ \nabla_{(\nu_1} \ldots \nabla_{\nu_m)} \varphi \right], \]

and the covariant Taylor series is simply

\[ |\varphi\rangle = P \sum_{n \geq 0} |n\rangle \langle n| \varphi\rangle. \]

The advantage of this machinery is that it allows us to take the familiar HDMS recursion relation:

\[ \left( 1 + \frac{1}{k} \sigma^\mu \nabla_\mu \right) a_k = \Delta^{-1/2} H(\Delta^{1/2} a_{k-1}) \equiv F a_{k-1}, \]

which follows from inserting the expansion Eq. (2) into Eq. (1) and give meaning to its formal solution

\[ a_k = P \left( 1 + \frac{1}{k} D \right)^{-1} \bar{F} \left( 1 + \frac{1}{k-1} D \right)^{-1} \bar{F} \cdots (1 + D)^{-1} \bar{F}, \]

(Where \( D \equiv \sigma \cdot \nabla \) and \( \bar{F} \equiv P^{-1} F P \)). This is accomplished by noting that \( D|n\rangle = n|n\rangle \), so that

\[ \left( 1 + \frac{1}{k} D \right)^{-1} = \sum_{n \geq 0} \frac{k}{k + n} |n\rangle \langle n|, \]

from which it follows that
\[ \langle n | a_k \rangle = \sum_{n_1, \ldots, n_{k-1} \geq 0} \frac{k}{k+n} \frac{k-1}{k-1+n} \cdots \frac{1}{1+n_1} \times \langle n | \tilde{F} | n_{k-1} \rangle \langle n_{k-1} | \tilde{F} | n_{k-2} \rangle \cdots \langle n_1 | \tilde{F} | 0 \rangle, \]  

with  

\[ \langle m | \tilde{F} | n \rangle = \left[ \nabla_{(\mu_1} \cdots \nabla_{\mu_m)} \tilde{F} \right] (-1)^n \frac{\sigma^{\nu_1} \cdots \sigma^{\nu_n}}{n!} \]

\[ = \left( \frac{m}{n} \right) \delta^{(\nu_1 \cdots \nu_n)}_{(\mu_1 \cdots \mu_m)} Z_{\mu_{n+1} \cdots \mu_m} - \left( \frac{m}{n-1} \right) \delta^{(\nu_1 \cdots \nu_{n-1} \mu_n)}_{(\mu_1 \cdots \mu_{m-1})} Y_{\mu_{n+1} \cdots \mu_m} \]

\[ + \left( \frac{m}{n-2} \right) \delta^{(\nu_1 \cdots \nu_{n-2} \mu_n)}_{(\mu_1 \cdots \mu_{m-2})} X_{\mu_{n+1} \cdots \mu_m} \]  

where  

\[ Z_{\mu_1 \cdots \mu_m} = (-1)^n \left[ \nabla_{(\mu_1} \cdots \nabla_{\mu_m)} Z \right], \]

\[ Y^{\nu}_{\mu_1 \cdots \mu_m} = (-1)^n \left[ \nabla_{(\nu_1} \cdots \nabla_{\nu_m)} Y^{\nu} \right], \]

\[ X^{\nu_1 \nu_2}_{\mu_1 \cdots \mu_m} = (-1)^n \left[ \nabla_{(\nu_1} \cdots \nabla_{\nu_2)} X^{\nu_1 \nu_2} \right]. \]

Here \( X, Y \) and \( Z \) are simply the coefficients of the Hamiltonian operator transported to the point \( x' \), that is  

\[ \tilde{F} = \mathcal{P}^{-1}(\mathcal{D}^{1/2} \Box \mathcal{D}^{-1/2} + Q) \mathcal{P} \]

\[ = \mathcal{P}^{-1} \mathcal{D}^{1/2} \nabla_{\mu'} \mathcal{D}^{-1} X^{\mu' \nu'} \nabla_{\nu'} \mathcal{D}^{1/2} \mathcal{P} + \bar{Q} \]

\[ = X^{\mu' \nu'} \nabla_{\mu'} \nabla_{\nu'} + Y^{\mu' \nu'} \nabla_{\mu'} + Z. \]  

### 3.1. Derivatives

Avramidi’s formalism is naturally adapted to computing the symmetrized derivatives of the \( a_k \), but frequently one requires the un-symmetrized derivatives. In order to obtain these, we can continue in the spirit of Avramidi and introduce matrix elements for the derivative operators. Defining  

\[ T_{\mu_1 \cdots \mu_m}^{\nu_1 \cdots \nu_n} [h_{\lambda_1} \cdots \lambda_n] = \langle 0 | \nabla_{\mu_1} \cdots \nabla_{\mu_m} \mathcal{P} h_{\lambda_1} \cdots \lambda_n | n \rangle, \]

we then have  

\[ [\nabla_{\nu_1} \cdots \nabla_{\nu_m} a_k] = \sum_{m} \frac{T_{\mu_1 \cdots \mu_m}^{\nu_1 \cdots \nu_m} [1]}{\langle m | a_k \rangle}. \]

Noting that  

\[ \nabla_{\mu} \mathcal{P} h_{\lambda_1} \cdots \lambda_n | n \rangle = -\mathcal{P} h_{\lambda_1} \cdots \lambda_n \eta^{(\nu_1\cdots \nu_n)} | n \rangle + \mathcal{P} \eta^{\nu_1} \cdots \nu_n \mathcal{A}_{\lambda_1} h_{\lambda_1} \cdots \lambda_n + \sum_{i} \mathcal{B}^{\mu} \lambda_1 \cdots \lambda_n | n \rangle \]

where \( \mathcal{B} \) is a special case of \( \mathcal{A} \): \( \mathcal{B}_{\sigma}^{\mu} = \frac{\partial}{\partial h_{\lambda_1}}, \) it is possible to derive a recursive expression for \( T \):  

\[ T_{\mu_1 \cdots \mu_m}^{\nu_1 \cdots \nu_n} [h_{\lambda_1} \cdots \lambda_i] = - \sum_{k=0}^{m-n-1} T_{\mu_1 \cdots \mu_{m-1}}^{\nu_1 \cdots \nu_{k+1} \cdots \nu_n} \cdot [\eta_{\mu_1 \cdots \mu_{m-1}}(\sigma^{\nu_1} \cdots \nu_{k+1} \cdots \nu_n) h_{\lambda_1} \cdots \lambda_n] \]

\[ + \sum_{k=1}^{m-n-1} T_{\mu_1 \cdots \mu_{m-1}}^{\nu_1 \cdots \nu_k} \cdot [\mathcal{A}_{\mu_1 \cdots \mu_{m-1}}(\sigma^{\nu_1} \cdots \nu_k) h_{\lambda_1} \cdots \lambda_n] \]

\[ + \sum_{k=1}^{m-n-1} \sum_{i=1}^{l} T_{\mu_1 \cdots \mu_{m-1}}^{\nu_1 \cdots \nu_k \cdots \nu_i} \cdot [\mathcal{B}_{\lambda_1}^{\sigma} \cdots \mu_1 \cdots \mu_{m-1} \cdots \nu_i h_{\lambda_1} \cdots \lambda_n]. \]
4. PROGRAM DESCRIPTION

4.1. Functions

The program implements most of the above functions, with the following correspondence:

\[ a_k = DCL[k], \]
\[ \nabla_{\mu_1} \ldots \nabla_{\mu_n} a_k = DCL[k, \mu_1, \ldots, \mu_n], \]
\[ X^{\alpha \beta}_{\nu_1 \ldots \nu_n} = XX[\alpha, \beta, \{\nu_1, \ldots, \nu_n\}], \]
\[ Y^\alpha_{\nu_1 \ldots \nu_n} = YY[\alpha, \{\nu_1, \ldots, \nu_n\}], \]
\[ Z_{\nu_1 \ldots \nu_n} = ZZ[\{\nu_1, \ldots, \nu_n\}], \]
\[ \nabla_{(\mu_1 \ldots \mu_n)} Q = QQ[\{\mu_1, \ldots, \mu_n\}], \]
\[ [Q] = QQ[ ], \]
\[ F^{\mu \nu} = F[\mu, \nu], \]
\[ R^{\mu \nu \alpha \beta} = R[\mu, \nu, \alpha, \beta]. \] (22)

In general, as already seen above, we use a list of bracketed indices to indicate symmetrized differentiation, so we also have for example

\[ \nabla_{(\mu_1 \ldots \mu_n)} F^{\alpha \beta} = F^{\alpha \beta}_{(\nu_1 \ldots \nu_n)} = F[\alpha, \beta, \{\mu_1, \ldots, \mu_n\}]. \] (23)

For completeness, we also list the following functions, although they are essentially internal functions:

\[ \langle m|F|n \rangle = MF[\{\nu_2, \ldots, \nu_n\}, \{\mu_1, \ldots, \mu_m\}], \]
\[ T_{\mu_1 \ldots \mu_m}^{\nu_1 \ldots \nu_n} [h_{\lambda_1 \ldots \lambda_n}] = MD[\{\nu_1, \ldots, \nu_n\}, \{\mu_1, \ldots, \mu_m\}, \{\lambda_1 \ldots \lambda_n\}, h_{\lambda_1 \ldots \lambda_n}], \] (24)

where we note that contrary to the convention, MD is not symmetric in the first set of indices.

4.2. Options

For the primary function \texttt{DCL} there are several options which control the normalization and degree of simplification. They are:

**HeatKNorm**

This controls the normalization that is used for the heat kernel coefficients returned by \texttt{DCL}. The default is Avramidi, which naturally invokes Avramidi’s normalization \((-1)^k/k!\). It can also be set to a function which should expect two arguments: the degree of the coefficient, and the number of derivatives.

**EvaluateK**

The curvature tensor occurs frequently through its symmetrized derivative \(K^{\alpha \beta(\nu)} = \nabla_{(\nu_1 \ldots \nu_n-2} R^{\alpha \nu_n-1 | \beta | \nu_n}).\) Setting this option to \texttt{True} expands \(K\) in terms of \(R\).

**EvaluateSymmetricDerivs**

Setting this to \texttt{True} means that objects such as \(Q[\{\nu_1, \ldots, \nu_n\}]\) will be expanded in terms of explicitly symmetrized derivatives (represented by the operator \texttt{Dx}), so that for example, \(Q[\{\mu_1, \mu_2\}] = (\text{Dx}[Q[ ], \mu_1, \mu_2] + \text{Dx}[Q[ ], \mu_2, \mu_1])/2.\)

**DoSimplifications**

This option controls whether derivatives will be re-ordered and other simplifications performed.

**DoBasicSimplifications**

This option controls whether to do basic simplifications like contracting indices. Setting this to \texttt{False} is really only useful when debugging.

There is also a global option defined for the \texttt{HeatK}:
EvaluateZZ

Setting this option to False means that ZZ, YY and XX will not be evaluated. This makes the results much more compact, though cryptic.

Two variables which describe the form of the derivative operator. The first, \$HeatKMetricStyle indicates whether one wishes to use the GR style metric diag(−1,1,1,...,1) or the HEP style metric diag(1,−1,...,−1). Setting it to −1 (the default) selects the former. The second variable, \$ScalarCurvatureFactor is used to include an explicit factor of the scalar curvature (\(R\)) into the Hamiltonian. For example, with \$HeatKMetricStyle = −1 and \$ScalarCurvatureFactor = −1/6, one has \(H = −\Box + Q − R/6\).

4.3. Examples

The following presents a simple example illustrating the use of the package, and showing how to change the settings to conform to various conventions. First load the package, assuming it is in the search path:

In[1]:= <<HeatK.m

By default, the package is set up to follow the sign and normalization conventions of Avramidi’s article. We can check that it reproduces those results.

In[2]:= a1 = DCL[1]

Out[2]= ZZ

In[3]:= a2 = DCL[2] // Expand

Out[3]= ZZ

In[4]:= a3 = DCL[3] // Expand

Out[4]= −YY ** ZZ

| \[\text{u1;(u2)}\] | \[\text{u1;(u2,2)}\] | \[\text{u1;u2)}\] |
|-------------------|-------------------|-------------------|
| \[\text{u1,1)}\] | \[\text{u1)}\] | \[\text{u1,2)}\] |

It is not difficult to see that the above results agree with those presented by Avramidi. Now, if we prefer, we can follow the conventions in his thesis.

In[5]:= \$HeatKMetricStyle = −1;
\[ In[6]:= a1 = DCL[1] \]
\[ Out[6]= ZZ ;() \]
\[ In[7]:= a2 = DCL[2] // Expand \]
\[ Out[7]= ZZ ;(u1,u1) ZZ ** ZZ + --------------- ;() ;() 3 \]
\[ In[8]:= a3 = DCL[3] // Expand \]
\[ Out[8]= -YY ** ZZ YY ** ZZ u1;(u2) ;(u1,u2) u1;(u2,u2) ;(u1) ------------------------ - ------------------------ + 3 4 ZZ ** ZZ ZZ ** ZZ ;() ;(u1,u1) ;(u1) ;(u1) ------------------- + ------------------ + 2 2 ZZ ** ZZ ;(u1,u1) ;() ------------------- + ZZ ** ZZ ** ZZ + 2 ;() ;() ;() XX ZZ ZZ u1,u2;(u3,u3) ;(u1,u2) ;(u1,u1,u2,u2) -------------------------- + ---------------- 6 10 \]

Now let’s now back up and see what some of these expressions are in more familiar notation. We can do this by changing the options for HeatK, allowing XX, YY and ZZ to be evaluated. We also switch back to the conventions in the nuclear physics article [1].

\[ In[9]:= SetOptions[HeatK, EvaluateZZ -> True]; \]
\[ $HeatKMetricStyle = -1; \]
\[ In[10]:= ZZ[] // ContractAll \]
\[ Out[10]= R QQ \]

\[ In[11]:= ZZ[u1, u1] // ContractAll // SimplifyCurvature // ReduceContractions \]
\[ Out[11]= -F ** F u1,u2 ** F u1,u2 R ;(u1,u1) ------------------------ + QQ ;(u1,u1) ---------------- + 2 2 \]

\[ SimplifyCurvature \] uses some tricks to put the curvature tensor into a "canonical" form, while \[ ContractAll \] and \[ ReduceContractions \] perform contractions, and simplify them - ZZ, XX and YY do not simplify their results, because they are usually not called directly.
We see that these results agree with Eqns. 3.83a and 3.83b of Ref. 1.

Now let’s compare with a standard reference, Barvinskii and Vilkovskii’s (BV) Physics Reports [4]. Avramidi defines his heat kernel coefficients with an explicit weight of \(1/k!\), so we have to divide by \(1/k!\) to get the more standard coefficients used by BV. Also, BV uses \((is)\) rather than \(t\) as the exponential parameter introduces an extra factor of \((-1)^k\) in their definition of the coefficients. All told, their conventions correspond to the following:

\[
\text{In}[12]:= \text{SetOptions[DCL, HeatKNorm} \rightarrow \((-1)^k/(#1)/(#1)!&\)];
\]
\[
$\text{HeatKMetricStyle} = -1; \ $\text{ScalarCurvatureFactor} = 1/6;
\]

We must also note that their matrix \(P\) is opposite in sign to Avramidi’s \(QQ\), so we correct for that as well.

\[
\text{In}[13]:= \text{DCL[1]} /. \_QQ \rightarrow -QQ
\]
\[
\text{Out}[13]= QQ
\]
\[
\text{In}[14]:= (a2 = \text{DCL[2]} // \text{Expand}) /. \_QQ \rightarrow -QQ
\]
\[
\text{Out}[14]= D D (QQ) D D (QQ) F ** F
\]
\[
\text{u1 u1 u1 u1 u1 u2 u1,u2 u1,u2 u1,u2 u1,u2,u3,u4}
\]
\[
\frac{1}{6} + \frac{2}{180} + \frac{2}{2} + \frac{3}{36}
\]
\[
\text{In}[15]:= \text{DCL[1, u1]} /. \_QQ \rightarrow -QQ
\]
\[
\text{Out}[15]= D (QQ) D (F )
\]
\[
\text{u1 u2 u1,u2}
\]
\[
\frac{1}{2} + \frac{6}{180}
\]
\[
\text{In}[16]:= \text{DCL[1, u1, u2]} /. \_QQ \rightarrow -QQ
\]
\[
\text{Out}[16]= D D (QQ) D D (F ) D D (F )
\]
\[
\text{u1 u2 u1 u2 u1 u3 u1,u3 u1 u3 u2,u3}
\]
\[
\frac{3}{12} + \frac{12}{12} + \frac{180}{60}
\]
\[
\text{D D (R) D D (R ) QQ ** F}
\]
\[
\text{u1 u2 u3 u1,u2 u1,u2}
\]
\[
\frac{3}{2} + \frac{12}{6}
\]
\[
\text{F ** QQ F ** F F ** F}
\]
\[
\text{u1,u2 u1,u3 u2,u3 u2,u3 u1,u3}
\]
\[
\frac{3}{12} + \frac{12}{12}
\]
\[
\text{R R F R}
\]
\[
\text{u1,u3 u2,u3 u3,u4 u1,u3,u2,u4}
\]
\[
\frac{3}{12}
\]
More Examples (as Mathematica notebooks) can be found at the WWW-site listed in the program summary.

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