A METHOD FOR CALCULATING THE HEAT KERNEL FOR MANIFOLDS WITH BOUNDARY

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The covariant technique for calculating the heat kernel asymptotic expansion for an elliptic differential second order operator is generalized to manifolds with boundary. The first boundary coefficients of the asymptotic expansion which are proportional to $t^{1/2}$ and $t^{3/2}$ are calculated. Our results coincide with completely independent results of previous authors.
1. Introduction

One of the most fruitful approaches in quantum field theory, especially in gauge theories and quantum gravity, is the approach of the effective action. It is applicable for topologically nontrivial manifolds (noncomplete manifolds with boundary etc.) as well. The effective action is calculable only within the limits of some perturbation theory. In general case of arbitrary background it is impossible to get an exact answer even in one-loop approximation. That is why one should use various approximate schemes for the investigation of various aspects of the effective action. One of the most important features of such calculational schemes should be manifest covariance of the calculations at each order.

The general framework of covariant methods for calculating the effective action is the heat kernel method [1]. Heat kernel plays very important role in quantum field theory. It has been successfully applied to the analysis of the structure of ultraviolet divergences and anomalies and renormalization [2] as well as to calculation of the finite part of the effective action that is expressible finitely in terms of the coefficients of the heat kernel asymptotic expansion.

Various methods for calculating heat kernel asymptotic expansion were developed [3-5]. However, most of them come to nothing more than manifolds without boundaries and can not be applied immediately to boundary problems.

Recently some papers dealing with boundaries appeared. These are, mainly, indirect methods that use the factorization properties of heat kernel and its behaviour under conformal transformations [6-8] or an expansion of the boundary in the neighbourhood of the tangent plane in some point [9,10]. On the other hand the general methods used in mathematical literature [11] are applicable in any case but the general covariance is lost and the method becomes not effective at higher orders. Nevertheless, the most complete summary of formulae concerning boundary contribution in heat kernel asymptotic expansion is presented in [6].

In this paper we propose a new algorithm for calculating boundary contributions in heat kernel asymptotic expansion. We show how the ordinary technique [1,4] can be applied for manifolds with boundary. A very close approach was developed in [12].

2. The general framework of calculations

Let $M$ be a $d$-dimensional compact riemannian manifold with smooth boundary $\partial M$, and $F$ be elliptic second order differential operator on $M$ of the form

$$F = -\Box + Q,$$

where $\nabla$ is a connection on smooth vector bundle $V$ over $M$ and $Q$ is an endomorphism of this bundle.

The heat kernel is defined by the equation

$$\left(\frac{\partial}{\partial t} + F\right) U(t|x,x') = 0,$$

where $\Box = g^{\mu\nu} \nabla_\mu \nabla_\nu$. 

(1)
with initial condition
\[ U(0|x, x') = g^{-1/2}(x)\delta(x, x') \] (3)

In the case of manifolds with boundary one should also impose suitable boundary conditions:
\[ BU(t|x, x') \bigg|_{x\in\partial M} = 0 \] (4)
Dirichlet
\[ B = 1 \] (5)
or Neumann ones
\[ B = (n^\mu\nabla_\mu + S) \] (6)
where \( n^\mu(x) \) is the unit inward pointing normal to the boundary and \( S \) is an endomorphism of the bundle \( V \).

In the case of compact manifolds without boundary conditions of periodicity are used instead of the boundary conditions (4). One can show that for any \( t > 0 \) the heat kernel is a smooth analytic function on the manifold \( M \), that behaves like a distribution (\( \delta \)-function) near the boundary.

In this paper we shall investigate the heat kernel, mainly, when the points \( x \) and \( x' \) are close together, as it is the limit \( x \to x' \) which is of interest in quantum field theory for calculating the effective action and vacuum expectation values of local observables.

Having in mind the calculation of heat kernel asymptotic expansion at \( t \to 0 \) let us take advantage of the quasi-classical approximation. Let us represent the solution of the equation (2) in the form
\[ U(t|x, x') = (4\pi t)^{-d/2}\Delta^{1/2}(x, x') \exp \left( -\frac{\sigma(x, x')}{2t} \right) \Omega(t|x, x') \] (7)
where \( \sigma(x, x') \) is a symmetric biscalar satisfying the equation
\[ \sigma = \frac{1}{2} \sigma_\mu\sigma^\mu = \frac{1}{2} \sigma_{\mu'}\sigma^{\mu'} , \] (8)
\[ \sigma_\mu = \nabla_\mu \sigma \quad \text{and} \quad \sigma_{\mu'} = \nabla_{\mu'} \sigma \]
and another biscalar \( \Delta(x, x') \) is defined by
\[ \Delta(x, x') = g^{-1/2}(x) \det (-\nabla_{\mu'}\nabla_\nu\sigma(x, x')) g^{-1/2}(x') \] (9)
and satisfies, as it is easy to show from (8), the equation
\[ \Delta^{-1/2}D\Delta^{1/2} = \frac{1}{2}(d - \Box \sigma) \] (10)

Making use of (2) and (7)-(10) we obtain a transfer equation for the function \( \Omega(t|x, x') \)
\[ \left( \frac{\partial}{\partial t} + \frac{1}{t} D + \Delta^{-1/2}F\Delta^{1/2} \right) \Omega(t|x, x') = 0 \] (11),
\[ D = \sigma^\mu \nabla_\mu \]

The initial and boundary conditions are to be determined from (3) and (5)-(6). But first let us discuss the general structure of this construction. As is generally known [1], the equation (8) determines the geodetic interval defined as one half the square of the length of the geodesic connecting the points \( x \) and \( x' \). However in general case of topologically nontrivial manifolds there are more than one geodesic between points \( x \) and \( x' \), i.e. the equation (8) has more than one solution. Therefore the quasi-classical ansatz, in general case, should have a form of a sum of analogous contributions from all geodesics. There is always one leading solution \( \sigma(x, x') \) which is determined by the shortest geodesic. It is marked out by the fact that it goes to zero

\[ [\sigma] \equiv \lim_{x \to x'} \sigma(x, x') = 0 \tag{12} \]

when the points \( x \) and \( x' \) approach each other. By the square brackets we denote here and below the coincidence limits of two-point quantities when the points \( x \) and \( x' \) tend to each other along the shortest geodesic.

If one fixes a sufficiently small region including the points \( x \) and \( x' \) (when they are close enough to each other) then only this single solution is left. Therefore it is in some sense local and does not depend on the global structure of the manifold. Multiple geodesics are closely associated with two reasons reflecting the essentially global (topological) aspects of the manifold. First, there could be manifolds with closed geodesics. In this case in addition to the shortest geodesic there are always geodesics that emanate from point \( x' \), pass through the whole manifold one or several times and return to the point \( x \). Second, geodesics could be reflected from boundaries of the manifold one or more times.

In general case there could be infinitely large number of additional geodesics. They can be ordered according to the value of the geodetic interval. It is obvious that the more times the geodesic is reflected from boundaries or passes through the whole manifold the larger the geodetic interval is. And according to (7) the value of the geodetic interval immediately determines the weight of the contribution of each geodesic in quasi-classical approximation. Let us mention that in heat kernel asymptotic expansion contribute only those geodesics for which the geodetic interval could vanish. (Note that in the euclidean signature used in this paper all the geodetic intervals are non-negative according to definition.) There is only one such a geodesic among all additional ones, namely, the geodesic with one reflection from the boundary. It is evident that it has the minimal geodetic interval in comparison with all others. Moreover, if one fixes sufficiently narrow strip of the manifold near the boundary including points \( x \) and \( x' \) then the geodesic with one reflection will be the only additional geodesic. In that sense the corresponding solution to the equation (8) is also local, i.e. it reflects the local properties of the boundary and does not depend on the global structure of the manifold. The corresponding geodetic interval \( \phi(x, x') \) in the coincidence limit \( x = x' \) equals doubled square of the normal distance to the boundary and, therefore, vanishes on the boundary

\[ [\phi] = 2r^2 \quad , \quad [\phi]_{\partial M} = 0 \tag{13} \]
Therefore the corresponding solution contributes in the heat kernel asymptotic expansion but only on the boundary. All other solutions to the equation (8) are essentially global and corresponding geodetic intervals are strictly positive and do not vanish anywhere. So for the analysis of the heat kernel asymptotic expansion it is sufficient to restrict oneself to the local term and the term with one reflection

$$ U(t) = (4\pi t)^{-t/2} \left( \exp \left( -\frac{\sigma}{2t} \right) \Delta^{1/2} \Omega(t) + \exp \left( -\frac{\phi}{2t} \right) \Psi(t) \right) $$  (14)

where $\Psi(t)$ is the corresponding transfer function. (Here it is convenient not to single out the pre-exponential factor, i.e the Van Vleck-Morette determinant.) The functions $\phi$ and $\Psi$ satisfy equations analogous to (8)-(11)

$$ \phi = \frac{1}{2} \phi_\mu \phi^\mu = \frac{1}{2} \phi_{\mu'} \phi^{\mu'} \quad , $$  (15)

$$ \phi_\mu = \nabla_\mu \phi \quad , \quad \phi_{\mu'} = \nabla_{\mu'} \phi $$

$$ L \Psi = 0 $$

$$ L = \frac{\partial}{\partial t} + \frac{1}{t} \left( \phi^{\mu} \nabla_\mu + \frac{1}{2} (\phi_\mu^{\mu'} - d) \right) - F $$  (16)

Since the second term in (14) does not contribute in the limit $t \to 0$ outside of the boundary and remembering that $[\Delta] = 1$ we get from (3) the initial condition for $\Omega$.

$$ [\Omega(0|x, x')] = 1 \quad . $$  (17)

The boundary conditions (4) take now the form:

Dirichlet

$$ \left( \Delta^{1/2} \Omega + \Psi \right) \bigg|_{x \in \partial M} = 0 $$  (18)

Neumann

$$ (n^\mu \nabla_\mu + S) \left( \Delta^{1/2} \Omega + \Psi \right) \bigg|_{x \in \partial M} - \frac{1}{2t} \sigma, n \left( \Delta^{1/2} \Omega - \Psi \right) \bigg|_{x \in \partial M} = 0 $$  (19)

where $\sigma, n = n^\mu \nabla_\mu \sigma$.

For calculating the function $\Omega$ it is sufficient to take advantage of the standard Schwinger-De Witt expansion

$$ \Omega(t) = \sum_{k=0}^{\infty} \frac{(-t)^k}{k!} a_k $$  (20)

where $a_k(x, x')$ are the so called Hadamard - Minakshisundaram - De Witt - Seeley coefficients (HMDS) which are determined completely independently of the boundary conditions by recursion relations

$$ \left( 1 + \frac{1}{k} D \right) a_k = \Delta^{-1/2} F \Delta^{1/2} a_{k-1} $$  (21)
The initial conditions for these recursion relations are obtained from (17) and have the form

\[ a_0 = 1 \]  \hspace{1cm} (22)

To solve these relations we have elaborated in the papers [4] a special technique. It allows to calculate an arbitrary HMDS-coefficient in a sufficiently effective way. It is shown there that the formal solution of the recursion relations (21)

\[ a_k = \left(1 + \frac{1}{k} D\right)^{-1} \Delta^{-1/2} F \Delta^{1/2} \left(1 + \frac{1}{k-1} D\right)^{-1} \Delta^{-1/2} F \Delta^{1/2} \cdots (1 + D)^{-1} \Delta^{-1/2} F \Delta^{1/2} \]  \hspace{1cm} (23)

takes the practical meaning in the form of covariant Taylor series

\[ a_k = \mathcal{P} \sum_{n \geq 0} \frac{(-1)^n}{n!} \sigma_{\mu_1} \cdots \sigma_{\mu_n} \left[ \nabla_{(\mu_1} \cdots \nabla_{\mu_n)} a_k \right] \]  \hspace{1cm} (24)

where \( \mathcal{P}(x, x') \) is the parallel displacement operator along the shortest geodesic from point \( x' \) to the point \( x \). In [4] the coefficients of that series are calculated and the results of calculations up to \( a_4 \) are listed. That is why we will concentrate our attention here on the calculation of the function \( \Psi \).

Let us choose for convenience of further calculations a special coordinate system in the neighbourhood of the boundary \( x^\mu = (r, \theta^i) \), where \( r \) is the length of the geodesic arc normal to the boundary in the point \( \theta \), the equation of the boundary having the form \( r = 0 \), and \( \theta^i \) are the normal riemannian coordinates on the boundary.

We assume all quantities to be analytic in the coincidence limit on the boundary \( \theta = \theta' \). Hence we will expand all quantities in covariant Taylor series in the neighbourhood of the boundary.

The further strategy is rather simple. One should introduce a small parameter reflecting the fact that parameter \( t \) is small and the points \( x \) and \( x' \) are close to each other and to the boundary

\[ t^{1/2} \sim r \sim r' \sim (\theta - \theta') \sim \varepsilon \]

and construct a corresponding perturbation theory in this parameter. We expand the transfer operator \( L \) (16) in a formal series in the small parameter \( \varepsilon \)

\[ L \left( \varepsilon^2 t | \varepsilon r, \varepsilon r', \varepsilon(\theta - \theta'), \theta' \right) = \frac{1}{\varepsilon^2} L_{-2} + \frac{1}{\varepsilon} L_{-1} + L_0 + \cdots \]  \hspace{1cm} (25)

and seek for a solution to this equation of the form

\[ \Psi \left( \varepsilon^2 t | \varepsilon r, \varepsilon r', \varepsilon(\theta - \theta'), \theta' \right) = \sum_{n \geq 0} \varepsilon^n \Psi_n \left( t | r, r', (\theta - \theta'), \theta' \right) \]  \hspace{1cm} (26)

From the transfer equation we get easy recursion differential relations

\[ L_{-2} \Psi_0 = 0 \]  \hspace{1cm} (27a)
\[ L_{-2} \Psi_1 = -L_{-1} \Psi_0 \]  \hspace{1cm} (27b)
\[ L_{-2} \Psi_2 = -L_{-1} \Psi_1 - L_0 \Psi_0 \]  \hspace{1cm} (27c)
etc..

One shows easily that the coefficients $\Psi_n$ satisfy the scaling properties

$$\Psi_n (\varepsilon^2 t | \varepsilon r, \varepsilon r', \varepsilon (\theta - \theta'), \theta') = \varepsilon^n \Psi_n (t | r', (\theta - \theta'), \theta')$$  \hspace{1cm} (28)

Analogous equations take place also for the function $\Omega$. Whereas these relations are sufficient for the calculation of all $\Omega_n$, for single-valued calculation of $\Psi_n$ it is necessary to use additionally the boundary conditions (18) (or (19)).

The main difference between them is that $\Omega_n$ are analytic in all variables while $\Psi_n$ are analytic in $$(\theta - \theta')$$ but are complicated functions of the variables $t$, $r$ and $r'$ (one can show that they are analytic in the variables $R = (r + r')$ and $u = (r - r')/(r + r')$, so that the point $r = r' = 0$ is singular).

Making use of the scaling property (28) one can get from (26) an important representation for $\Psi(t)$

$$\Psi (t | r, r', (\theta - \theta'), \theta') = \sum_{n \geq 0} r^{n/2} \Psi_n \left( \frac{r}{\sqrt{t}}, \frac{r'}{\sqrt{t}}, (\theta - \theta'), \theta' \right)$$  \hspace{1cm} (29)

Using (11) and (14) we write down for the trace of the heat kernel

$$Tr [f U(t)] = \int_M dx g^{1/2} Tr [f U(t)] =$$

$$= (4\pi t)^{-d/2} tr \left\{ \int_M dx g^{1/2} [f \Omega(t)] + \int_{\partial M} d\theta \gamma^{1/2} \int_0^\infty dr \exp \left( -\frac{r^2}{t} \right) \frac{g^{1/2}}{\gamma^{1/2}} [f \Psi(t)] \right\}$$  \hspace{1cm} (30)

where $f(x)$ is an arbitrary smooth function on the manifold and $\gamma = \det \gamma_{ij}$, $\gamma_{ij}$ is the induced metric on the boundary. One should mention that additional terms due to the presence of the boundary contribute to the asymptotic expansion of the trace of the heat kernel at $t \to 0$ only when integrating over a sufficiently narrow neighbourhood of the boundary. Therefore, the upper limit of the integration over the distance to the boundary $r$ in (30) is taken to be $\infty$ (up to exponentially small terms).

At last, using (20) and (29) we obtain the asymptotic expansion of the trace of the heat kernel both in volume part and in surface one)

$$Tr fU(t) = (4\pi t)^{-d/2} tr \left\{ \int_M dx g^{1/2} \sum_{k=0}^\infty \frac{(-t)^k}{k!} [f a_k] + \int_{\partial M} d\theta \gamma^{1/2} \sum_{k=0}^\infty \frac{t^{k+1}}{2} c_{k+1}(f) \right\}$$  \hspace{1cm} (31)

where

$$c_{k+1}(f) = \sum_{0 \leq m \leq n} \int_0^\infty d\xi \exp (-\xi^2) \xi^m b_{k-n} (\xi) \sum_{0 \leq m \leq n} \frac{g_m}{m!} \frac{f^{(n-m)}}{(n-m)!}$$  \hspace{1cm} (32a)

$$b_k(\xi) = t^{-k/2} \Psi_k \bigg|_{r=\xi \sqrt{t}}$$  \hspace{1cm} (32b)

$$f^{(k)} = \mu_1 \cdots \mu_k \nabla_{\mu_1} \cdots \nabla_{\mu_k} f \bigg|_{r=0}$$
Thus for the calculation of the boundary contributions in heat kernel asymptotic expansion one suffices to compute the coincidence limits $\lbrack \Psi_n \rbrack$, put $t = 1$, integrate with the weight $\exp(-r^2)r^m$ and combine them with the quantities $g_k$ (33) calculated before.

3. Explicit expressions

Here we list the results of calculations of the lower order coefficients of the heat kernel asymptotic expansion omitting most of the cumbersome computations. The most complete list of volume contributions $a_k$ is presented in [4]. The simplest first of them have the form

\begin{align*}
[a_0] &= 1 \\
[a_1] &= Q - \frac{1}{6} R \\
[a_2] &= \left( Q - \frac{1}{6} R \right)^2 - \frac{1}{3} \Box Q - \frac{1}{90} R_{\mu\nu} R^{\mu\nu} + \frac{1}{90} R_{\mu\nu\alpha\beta} R^{\mu\nu\alpha\beta} + \frac{1}{15} \Box R + \frac{1}{6} R_{\mu\nu} R^{\mu\nu}
\end{align*}

where $R_{\mu\nu} = [\nabla_\mu, \nabla_\nu]$.

Using the set of normal coordinates introduced above it is not difficult to calculate the coefficients $g_k$ (33)

\begin{align*}
g_0 &= 1 \\
g_1 &= -K \\
g_2 &= -K_{ij} K^{ij} + K^2 - R^0_{nn}
\end{align*}

where

\begin{align*}
K &= \gamma^{ij} K_{ij} \\
K_{ij} &= -\frac{1}{2} \frac{\partial}{\partial r} g_{ij} \bigg|_{r=0} \\
\gamma_{ij} &= g_{ij} \bigg|_{r=0} \\
R^0_{nn} &= n^\mu n^\nu R_{\mu\nu} \bigg|_{r=0}
\end{align*}

For simplicity we list below the solution only for Dirichlet boundary conditions. From equation (27) and boundary condition (18) we have

\begin{equation}
\Psi_0 = -1
\end{equation}
The calculation of next orders is considerably more difficult though it offers no particular problems. The result has the form

\[ [\Psi_1] = \sqrt{t} \left\{ -\frac{r^2}{t} h \left( \frac{r}{\sqrt{t}} \right) K \right\} \]

\[ [\Psi_2] = t \left\{ \left( Q - \frac{1}{6} \hat{R} \right) - \frac{1}{3} \left( 1 + \frac{r^2}{t} \right) R^0_{nn} \right. \]

\[ \left. + f_1 \left( \frac{r}{\sqrt{t}} \right) K^2 + f_2 \left( \frac{r}{\sqrt{t}} \right) K_{ij} K^{ij} \right\} \] (37)

where all tensor quantities are calculated on the boundary and \( \hat{R} \) is the scalar curvature of the boundary

\[ h(z) = \int_0^\infty dx \exp(-x^2 - 2zx) = \exp(z^2)Erfc(z) \]

\[ f_1(z) = \frac{1}{6} + \frac{z^2}{6} \left( 2 + \frac{1}{2} z^2 - z(z^2 + 6) h(z) \right) \]

\[ f_2(z) = -\frac{1}{6} + \frac{1}{12} z^2 \left( -4 + \frac{1}{2} z^2 - 4z^3 h(z) \right) \] (38)

Using these expressions and the integrals

\[ \int_0^\infty \exp(-\xi^2)\xi^n h(\xi) = \frac{\Gamma \left( \frac{n+2}{2} \right)}{2(n+1)} \]

we get finally several first boundary coefficients in asymptotic expansion (31)

\[ c_{1/2}(f) = -\frac{\sqrt{\pi}}{2} \]

\[ c_1(f) = \frac{1}{3} K - \frac{1}{2} f^{(1)} \]

\[ c_{3/2}(f) = \frac{\sqrt{\pi}}{2} \left\{ \left( -\frac{1}{6} \hat{R} - \frac{1}{4} R^0_{nn} + \frac{3}{32} K^2 - \frac{1}{16} K_{ij} K^{ij} + Q \right) f \right. \]

\[ \left. + \frac{5}{16} K f^{(1)} - \frac{1}{4} f^{(2)} \right\} \] (39)

These results coincide with ones obtained by completely independent methods in [6] that confirms that the approach developed in this paper is correct.

Obtained results may be used when investigating Green function and the energy-momentum tensor of quantum fields near the boundary.

3. Conclusion
In this paper a new method for calculating the heat kernel asymptotic expansion (or one-loop effective action in any model of field theory) in the case of arbitrary background fields and manifolds of nontrivial topology (with boundary) is proposed. This method is a generalization of our previously elaborated covariant technique for calculation of the effective action and is based on the summation in the quasi-classical approximation the contributions of all geodesics connecting any two points of the manifold (including the geodesics reflected from the boundary). It is established that taking into account one additional geodesic with single reflection correctly reproduces all boundary contributions in the heat kernel asymptotic expansion. Proposed approach allows not only to calculate the asymptotic expansion of the trace of the heat kernel but also to analyze the local structure of the heat kernel near the boundary. Furthermore we are going to calculate by means of it also the next terms of the asymptotic expansion $\sim t^2$ and $\sim t^{5/2}$, i.e. the coefficients $c_2$ and $c_{5/2}$.

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