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1999 J. Phys. A: Math. Gen. 32 8247

(http://iopscience.iop.org/0305-4470/32/47/304)

J. Phys. A: Math. Gen. **32** (1999) 8247–8259. Printed in the UK PII: S0305-4470(99)06039-4

Heat kernel expansion for semitransparent boundaries

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Received 15 July 1999

Abstract. We study the heat kernel for an operator of Laplace type with a δ-function potential concentrated on a closed surface. We derive the general form of the small t asymptotics and explicitly calculate several first heat kernel coefficients.

1. Introduction

Singular potentials are a frequently used idealization of physical situations allowing for an easier (and, sometimes, explicit) solution while keeping the essential features of the problem. The best studied cases of singular potentials are the δ function potentials concentrated at isolated points, which describe the contact interactions of particles (for a review, see [1]). Rigorous analysis of such potentials was initiated by Berezin and Faddeev [2] and has since developed in a mature mathematical discipline [1]. Additional cases of singular potentials also include cosmic strings and other topological defects [3], and problems related to black hole entropy [4]. We also wish to mention a recent work on the boundary discontinuities [5].

With respect to the Casimir effect, a δ function shaped potential provides the simplest generalization of the conductor boundary conditions moving towards the inclusion of more realistic properties of the walls, such as partial transparency. For a scalar and a spinor field with plane boundaries this problem has been investigated in [6], and for moving partly transmitting mirrors in [7]. An interesting approach using 'semihard' and 'weak' boundaries is developed in [8]. In all these cases it is crucial to know the ultraviolet divergences in order to find the structure of the necessary counterterms. This is equivalent to the investigation of the corresponding heat kernel asymptotics. As is known [9], this is an expansion with respect to integer powers of the proper time parameter t (see below) for Laplace-type operators on closed manifolds and to half-integer powers, i.e. to powers of $\sqrt{t}$, on manifolds with boundaries and Dirichlet or Robin boundary conditions. For more complicated pseudo-differential operators powers of $\ln t$ may appear.

This paper is devoted to singularities which are located on closed hypersurfaces of dimension $m-1$, where m is the dimension of the underlying manifold. Apart from the quantum mechanical problem of a particle in space with semitransparent boundaries (for a recent calculation of the vacuum energy for such a system see, for example, [10]) possible physical applications also include fermions on the background of a magnetic tube [11] and

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photons interacting with dielectric bodies [12,13]. In all these cases the dynamics is described by a second-order differential operator of Laplace type, supplemented by certain matching conditions on a surface. Our primary interest is in the heat kernel asymptotics. They govern the short-time asymptotics of quantum mechanical propagators, the ultraviolet divergences and the large-mass expansion in quantum field theory.

The heat kernel coefficients for singular potentials cannot be obtained, in general, as limiting cases of smooth configurations. This is already clear from the fact that the heat kernel expansion for a smooth potential contains powers of the potential taken at the same point. Such expressions become ill-defined in the δ function limit. In the paper by Kirsten and the present authors [13], the suprising property was observed that sometimes the ultraviolet behaviour of a system with δ-function potential is less singular than that of corresponding 'smooth' system.

Let us proceed with basic definitions. Let M be a smooth Riemannian manifold of dimension m. Let Σ be a smooth closed submanifold of co-dimension 1. Let $\mathcal{V}$ be a vector bundle over M. Let E and V be endomorphisms of $\mathcal{V}$ and $\mathcal{V}|_\Sigma$, respectively. In a more 'physical' language, E and V are matrix valued functions bearing spin and internal indices. In this paper we study the heat kernel expansion for the operator

$$D = -(\nabla^2 + E(x) + \delta_\Sigma V(x)) = D_0 - \delta_\Sigma V(x). \tag{1}$$

Let $\mathrm{d}x$ and $\mathrm{d}y$ be the Riemannian volume elements on M and Σ. We normalize the δ_Σ function in such a way that for any smooth function f

$$\int_M \delta_\Sigma f(x)\,\mathrm{d}x = \int_\Sigma f(y)\mathrm{d}y. \tag{2}$$

We adopt the following short-hand notation for the integrals:

$$\int_M \mathrm{d}x\,F(x) = \{F\}[M] \qquad \int_\Sigma \mathrm{d}y\,F(y) = \{F\}[\Sigma]. \tag{3}$$

We can choose the coordinates in such a way that in the vicinity of Σ the metric has the form

$$g_{ij}\mathrm{d}x^i\,\mathrm{d}x^j = (\mathrm{d}x^m)^2 + g_{ab}\,\mathrm{d}x^a\,\mathrm{d}x^b. \tag{4}$$

The second fundamental form of Σ is $L_{ab} = \frac{1}{2}\partial_m g_{ab}$. We suppose that $x^m = 0$ on Σ. Our notation is the same as in [14]. R_{ijkl} are the components of the Riemann curvature tensor. With our sign conventions, R_{1212} is negative on the standard sphere in Euclidean space. The Ricci tensor ρ and the scalar curvature τ are given by

$$\rho_{ij} := R_{ikkj} \qquad \tau = \rho_{ii} = R_{ikki}. \tag{5}$$

Let $\rho^2 := \rho_{ij}\rho_{ij}$ and $R^2 := R_{ijkl}R_{ijkl}$ be the norm of the Ricci and full curvature tensors. Let Ω_{ij} be the endomorphism-valued components of the curvature of the connection on $\mathcal{V}$. In physical language, Ω_{ij} is the field strength for the Yang–Mills and spin connections. Let ';' denote multiple covariant differentiation with respect to the Levi-Civita connection of M, and let ':' denote multiple tangential covariant differentiation on Σ with respect to the Levi-Civita connection of Σ; the difference between these two is measured by the second fundamental form. For example, $f_{;jj} = f_{;mm} + f_{;aa} = f_{;mm} + f_{:aa} - L_{aa} f_{;m}$.

A mathematically rigorous way to define the spectral problem for the operator D is to replace it by the spectral problem for D_0 for $x \notin \Sigma$ supplemented by the conditions on Σ (see, for example, [1]):

$$\phi(-0) = \phi(+0) \tag{6}$$

$$\nabla_m\phi(-0) - \nabla_m\phi(+0) = V\phi(0) \tag{7}$$

with the short-hand notation $\phi(\pm 0) = \lim_{x^m\to\pm 0}\phi(x)$.

The heat kernel $K(x, y; t)$ is a solution of the heat equation

$$(\partial_t + D_0)K(x, y; t) = 0 \tag{8}$$

with the initial condition

$$K(x, y; 0) = \delta(x, y) \tag{9}$$

which satisfies the matching conditions on Σ following from (6) and (7).

We are interested in the integrated heat kernel

$$K(f, D; t) = \{f(x)K(x, x; t)\}[M] = \mathrm{Tr}(f \exp(-tD)). \tag{10}$$

On manifolds with local boundary conditions there is an asymptotic expansion as $t \to +0$

$$K(f, D; t) = \sum_{n\geqslant 0} a_n(f, D)t^{(n-m)/2} \tag{11}$$

where the coefficients $a_n(f, D)$ are volume and surface integrals of local invariants. The existence of the asymptotic expansion (11) is usually considered as granted. There are, however, important exceptions (besides 'genuine' pseudo-differential operators, the square root of the Laplacian, for instance), such as the boundary value problem for spectral boundary conditions, and δ-function potentials with point-like support on manifolds with dimension $m \geqslant 2$. In such cases $\ln t$ terms can appear in the asymptotic expansion [15–17]. To the best of our knowledge, the existence of expansion (11) for the problem considered here has never been stated before.

This paper is organized as follows. In the next section we derive an integral equation for the heat kernel and show the validity of the asymptotic expansion (11). In section 3 we calculate the heat kernel asymptotics for the particular case when Σ is a sphere in $\mathbb{R}^m$. In section 4 we derive explicit expressions for the heat kernel coefficients $a_n(f, D)$, $n \leqslant 5$, for the most general form of the operator D. To this end, we use the particular case calculations of section 3 and functorial properties of the heat kernel.

2. General structure of the heat kernel

To study the general structure of the heat kernel expansion we use an integral equation similar to that proposed by Gaveau and Schulman [18] for the one-dimensional δ-potential:

$$K(x, y; t) = K_0(x, y; t) + \int_0^t \mathrm{d}s \int_\Sigma \mathrm{d}z\, K_0(x, z; t-s)V(z)K(z, y; s) \tag{12}$$

where $K_0(x, y; t)$ denotes the heat kernel corresponding to the operator D_0 with $V = 0$.

Equation (12) has a solution in the form of the power series in V:

$$K(x, y; t) = K_0(x, y; t) + \sum_{n=1}^{\infty} \int_0^t \mathrm{d}s_n \int_0^{s_n} \mathrm{d}s_{n-1} \ldots \int_0^{s_2} \mathrm{d}s_1 \int_\Sigma \mathrm{d}z_n \ldots \int_\Sigma \mathrm{d}z_1 \\ \times K_0(x, z_n; t-s_n)V(z_n)K_0(z_n, z_{n-1}; s_n - s_{n-1}) \ldots V(z_1)K_0(z_1, y; s_1). \tag{13}$$

Equation (12) can be obtained formally as a limiting case of the smooth potential. Instead of investigating this limiting procedure we prefer to directly check that the heat kernel defined by (12) satisfies the heat equation (8) with the initial condition (9) and boundary conditions which follow from (6) and (7). The initial condition (9) is evident from the equation (13). Only the first term contributes at $t = 0$ if $x, y \notin \Sigma$. The heat equation (8) can be checked by a direct calculation. The first of the matching conditions (6) merely expresses the fact that the heat kernel $K_0(x, y; t)$ is smooth enough. The second condition (7) is a bit less trivial. Let $y \notin \Sigma$. Then the following sequence of transformations holds:

$$\begin{aligned}
&\nabla_m^x K(-0, y; t) - \nabla_m^x K(+0, y; t) \\
&\quad = -\lim_{\epsilon\to 0} \int_{-\epsilon}^{\epsilon} \mathrm{d}x^m\, \nabla_m^2 \int_0^t \mathrm{d}s \int_\Sigma \mathrm{d}z\, K_0(x, z; t-s) V(z) K(z, y; s) \\
&\quad = \lim_{\epsilon\to 0} \int_{-\epsilon}^{\epsilon} \mathrm{d}x^m\, D_0^x \int_0^t \mathrm{d}s \int_\Sigma \mathrm{d}z\, K_0(x, z; t-s) V(z) K(z, y; s) \\
&\quad = \lim_{\epsilon\to 0} \int_{-\epsilon}^{\epsilon} \mathrm{d}x^m \int_0^t \mathrm{d}s \int_\Sigma \mathrm{d}z\, (\partial_s K_0(x, z; t-s)) V(z) K(z, y; s) \\
&\quad = \lim_{\epsilon\to 0} \int_{-\epsilon}^{\epsilon} \mathrm{d}x^m \int_0^t \mathrm{d}s \int_\Sigma \mathrm{d}z\, K_0(x, z; t-s) V(z) D_0^y K(z, y; s) \\
&\qquad + \lim_{\epsilon\to 0} \int_{-\epsilon}^{\epsilon} \mathrm{d}x^m \int_\Sigma \mathrm{d}z\, [\delta(x, z) V(x) K(z, y; t) - K_0(x, z; t) V(z) \delta(z, y)] \\
&\quad = V(x^a, 0) K((x^a, 0), y; t).
\end{aligned}$$

The main advantage of representation (13) is that the small-t behaviour of $K(x, y; t)$ is defined through the small-t behaviour of $K_0(x, y; t)$ which is known in some detail. To simplify notation we do not explicitly write down the volume elements here, or the parallel transport matrices later on. We also drop all matrix indices.

We are interested in the integrated heat kernel $K(t) = \int \mathrm{d}x\, K(x, x; t)$, where we put the smearing function $f = 1$ for simplicity. The integration over x can be performed by using the equation

$$\int_M \mathrm{d}x\, K_0(x, y_1; \tau_1) K_0(y_2, x; \tau_2) = K_0(y_1, y_2; \tau_1 + \tau_2) \tag{14}$$

which follows from the evident operator identity $\mathrm{e}^{-\tau_1 D_0}\mathrm{e}^{-\tau_2 D_0} = \mathrm{e}^{-(\tau_1+\tau_2)D_0}$. We have

$$\begin{aligned}
K(t) = K_0(t) + \sum_{n=1}^{\infty} \int_0^t \mathrm{d}s_n \int_0^{s_n} \mathrm{d}s_{n-1} \ldots \int_0^{s_2} \mathrm{d}s_1 \int_\Sigma \mathrm{d}z_n \ldots \int_\Sigma \mathrm{d}z_1 \\
\times K_0(z_1, z_n; t + s_1 - s_n) V(z_n) K_0(z_n, z_{n-1}; s_n - s_{n-1}) \ldots V(z_1).
\end{aligned} \tag{15}$$

It is instructive to explicitly calculate several of the first terms of expansion (15). In the linear order in V, one immediately gets

$$K_1(t) = t \int_\Sigma \mathrm{d}z\, K_0(z, z; t) V(z). \tag{16}$$

This equation means that the liner order in V can be obtained from the asymptotic expansion for the heat kernel in which a smooth potential is replaced by the singular one. Such a simple relation does not hold at higher orders in V.

In analysing the order-V^2 contributions we suppose that D_0 is just the standard scalar Laplacian in $\mathbb{R}^m$, neglect derivatives of V and suppose that Σ is flat. However, we turn to a slightly more general case and allow Σ to be of dimension $m - k$. In this particular case $K_0(x, y; t) = (4\pi t)^{-m/2} \exp(-(x - y)^2/4t)$ and

$$K_2(t) = (4\pi)^{-\frac{m+k}{2}} t^{\frac{m-k}{2}} \int_\Sigma \mathrm{d}z\, V(z)^2 \int_0^t \mathrm{d}s_2 \int_0^{s_2} \mathrm{d}s_1\ ((t - s_2 + s_1)(s_2 + s_1))^{-\frac{k}{2}}\,. \tag{17}$$

For $k > 1$ the integrals over s are divergent. This shows that the proposed method cannot be extended, particularly for $\delta(r)$ potentials in $\mathbb{R}^m$ with $m \geqslant 2$, for which expansion (11) is known to break down [16, 17]. We now return to the subject of our study, $k = 1$. All integrals are easily calculated giving

$$K_2(t) = \frac{t}{(4\pi t)^{(m-1)/2}} \frac{1}{8} \int_\Sigma \mathrm{d}z\, V(z)^2 + \cdots \tag{18}$$

where we have omitted all higher-order terms.

To calculate the other terms in expansion (15) one can use the following strategy. Let us substitute the small-s asymptotic expansion for the $K_0(x, y; s)$

$$K_0(x, y; s) \sim \frac{\exp(-\sigma(x, y)/2s)}{(4\pi s)^{m/a}} \left(A_0^{(0)}(x, y) + s A_2^{(0)}(x, y) + \cdots\right) \tag{19}$$

where $\sigma(x, y)$ is the half square of the geodesic distance between x and y; $A_{2i}^{(0)}(x, y)$ are the heat kernel coefficients for the operator D_0. Contributions to (15) of largely separated points are exponentially damped. Therefore, we may expand $A_{2i}^{(0)}(z_j, z_{j-1})$ and $\sigma(z_j, z_{j-1})$ in Taylor series in $(z_j - z_{j-1})$. The potentials $V(z_j)$ are to be expanded around a certain point, say z_1. Finally, the expression given under the integrals in (15) will become a sum of the monomials

$$\exp\left(-\frac{(z_1 - z_n)^2}{4(t - s_1 + s_n)} - \cdots - \frac{(z_2 - z_1)^2}{4(s_2 - s_1)}\right) I^{(N)}(V, \ldots; z_1) \frac{(z_1 - z_n)^{N_1}}{(t - s_1 + s_n)^{M_1}} \cdots \frac{(z_2 - z_1)^{N_n}}{(s_2 - s_1)^{M_n}} \tag{20}$$

where $I^{(N)}$ is a local invariant functional of V, geometric invariants and their derivatives calculated at the point z_1. Negative powers of $(s_j - s_{j-1})$ appear due to the expansion of the $\sigma(z_j - z_{j-1})$ in the exponentials. It is easy to see that $M_j \leqslant N_j/2$.

Integrals over z_i, except for the last one over z_1, can be calculated with the help of the relation

$$\int_{\mathbb{R}^n} \mathrm{d}x\, \exp\left(-\frac{(y_1 - x)^2}{4\alpha} - \frac{(x - y_2)^2}{4\beta}\right) = \left(\frac{4\pi\alpha\beta}{\alpha + \beta}\right)^{\frac{n}{2}} \exp\left(-\frac{(y_1 - y_2)^2}{4(\alpha + \beta)}\right) \tag{21}$$

with positive real parameters α and β. Note that equation (21) is just a particular case of (14) when D_0 is the flat space Laplacian. Integrals of even powers of $(x - y_1)$ with the same exponential weight are obtained by differentiation of (21) with respect to α. Odd powers of x can be integrated by using the following obvious relation:

$$\int_{\mathbb{R}^n} \mathrm{d}x\, \left(x^a - \frac{\beta y_1^a + \alpha y_2^a}{\alpha + \beta}\right) \exp\left(-\frac{(y_1 - x)^2}{4\alpha} - \frac{(x - y_2)^2}{4\beta}\right) = 0. \tag{22}$$

Before integrating over s_j let us introduce rescaled variables $\tilde{s}_j = s_j/t$. This enables us to extract an overall power of the proper time t. Integrals over $\tilde{s}_j$ will only give numerical factors. One can easily see that the strongest possible singularity of the integrand has the form $((1 - \tilde{s}_n + \tilde{s}_1) \ldots (\tilde{s}_2 - \tilde{s}_1))^{-\frac{1}{2}}$. This singularity is integrable. Hence the integral over $\tilde{s}_j$ always exists. After all the integrations have been performed one obtains $\int_\Sigma \mathrm{d}z_1\, I^{(N)}(V, \ldots; z_1)$ multiplied by a numerical coefficient and a power of $\sqrt{t}$.

Generalization of the procedure proposed in this section for the case of the non-unit smearing function f is obvious. Therefore, we have demonstrated that for the spectral problem considered in this paper the asymptotic expansion (11) is valid where the coefficients $a_n(f, D)$ are integrals over M and Σ of local invariants. Volume terms are the same as in the heat kernel expansion for the operator D_0.

3. Penetrable spherical shell

Before calculating the heat kernel expansion for the generic form of the operator D, consider a particular case of the constant potential V with the support on a spherical shell of the radius R:

$$V(x)\delta_\Sigma = -\frac{\alpha}{R}\delta(r-R). \tag{23}$$

Here r is the radial coordinate. Let D_0 in (1) be the standard scalar Laplacian in $\mathbb{R}^m$. After separating the angular variables the eigenvalue equation takes the form

$$\left(-\frac{\partial^2}{\partial r^2} - \frac{(m-1)}{r}\frac{\partial}{\partial r} + \frac{l(l+m-2)}{r^2}\right)\phi = k^2\phi \tag{24}$$

where $l = 0, 1, 2, \ldots$ is the orbital momentum. After the substitution $\phi(r) = r^{(2-m)/2}\psi(r)$ the equation takes the form

$$\left(-\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \frac{\nu^2}{r^2}\right)\psi = k^2\psi \tag{25}$$

where the notation $\nu = l + \frac{m-2}{2}$ is introduced.

The basic ideas of the formalism used in this section are contained in [19]. The zeta function associated with this operator can be written in the form

$$\zeta(s) = \int_0^\infty \frac{\mathrm{d}t}{t}\frac{t^s}{\Gamma(s)} K(t) \tag{26}$$

where $K(t)$ is the integrated heat kernel. The function $\Gamma(s)\zeta(s)$ has simple poles in $s = \frac{d}{2} - N$ ($N = 0, \frac{1}{2}, 2, \ldots$) whose residua are determined by expansion (11) of the heat kernel for $t \to 0$. It can be easily seen that the coefficients are related to the residua by means of

$$a_n = \mathrm{Res}_{s=\frac{m-n}{2}}\,\Gamma(s)\zeta(s). \tag{27}$$

These heat kernel coefficients can be obtained by calculating the zeta function starting from the differential equation (25). The zeta function of the operator D can be expressed in the form

$$\zeta(s) = \frac{\sin\pi s}{\pi}\sum_{l=0}^\infty D_l \int_0^\infty \mathrm{d}k k^{-2s}\frac{\partial}{\partial k}\ln f_l(\mathrm{i}k) \tag{28}$$

where $f_l(k)$ is the Jost function of the scattering problem corresponding to the operator D and

$$D_l = \frac{(2l+m-2)\,(l+m-3)!}{l!\,(m-2)!} \qquad m \geqslant 3 \tag{29}$$

is the multiplicity of the orbital eigenvalues. This representation, as it stands, is valid for $\mathrm{Re}\, s > \frac{m}{2}$. The Jost function reads [13]

$$f_l(\mathrm{i}k) = 1 + \alpha I_\nu(k)K_\nu(k). \tag{30}$$

In equation (28) the contribution resulting from the empty space (it is independent from α) is dropped. Due to this reason there is no contribution corresponding to the coefficient a_0 there.

In fact, we need the residua of the function $\Gamma(s)\zeta(s)$. These are delivered when inserting the uniform asymptotic expansion for $k \to \infty$ and $l \to \infty$ of the Jost function into equation (28). The latter can be obtained simply by inserting the known expansions of the Bessel functions into (30). This expansion can be written in the form

$$\ln f_l(\mathrm{i}k) = \sum_{n,i} X_{n,i} t^i \nu^{-n}. \tag{31}$$

Here, $n = 1, \ldots, N_m$, and N_m is the number of the highest heat kernel coefficient requiring calculation. The coefficients $X_{n.i}$ are numbers, some of the first appearing in (31) are given in the appendix. The notation $t = \sqrt{1 + (k/\nu)^2}$ is used. When inserting (31) into the rhs of equation (28), the change of variables $k \to \nu k$ can be made after which the expression factorizes. The integral can be calculated easily. It reads

$$\int_0^\infty \mathrm{d}k k^{-2s} \frac{\partial}{\partial k} t^i = -\frac{\Gamma(1-s)\Gamma(s+\mathrm{i}/2)}{\Gamma(\mathrm{i}/2)}. \tag{32}$$

The sum over l takes the form

$$\zeta(d, n) = \sum_{l=0}^\infty D_l \nu^{-2s-n}. \tag{33}$$

The functions $\zeta(d, n)$ can be expressed in terms of Riemann and Hurwitz zeta functions. They are shown in the appendix.

Now the heat kernel coefficients can be expressed in the form

$$a_N = -\operatorname{Res}_{s=\frac{d-N}{2}} \sum_{n=1}^{N_m} \zeta(d, n) \sum_i X_{n,i} \frac{\Gamma(s+\mathrm{i}/2)}{\Gamma(\mathrm{i}/2)} \qquad \left(N = 1, \tfrac{3}{2}, 2, \tfrac{5}{2}, \ldots, N_m\right). \tag{34}$$

The sum over i runs from $i = n$ to $i = n + 4([\frac{n+1}{2}] - 1)$ where $[\ldots]$ denotes the integer part. In this form they can be calculated immediately using one of the standard computer systems for analytical calculations. As a result, we obtain that $a_1 = 0$ in any dimension. For $m = 3$ other coefficients read:

$$\begin{aligned} a_2 &= \frac{-\alpha}{2\sqrt{\pi}} & a_3 &= \frac{\alpha^2}{8} \\ a_4 &= \frac{-\alpha^3}{12\sqrt{\pi}} & a_5 &= \frac{\alpha^4}{64} \\ a_3 &= \frac{-(\alpha^3(4+21\alpha^2))}{2520\sqrt{\pi}} & a_7 &= \frac{\alpha^4(1+2\alpha^2)}{1536} \end{aligned} \tag{35}$$

for $m = 4$:

$$\begin{aligned} a_2 &= \frac{-\alpha}{8} & a_3 &= \frac{\alpha^2\sqrt{\pi}}{32} \\ a_4 &= \frac{-\alpha^3}{48} & a_5 &= \frac{-(\alpha^2(3-4\alpha^2)\sqrt{\pi})}{1024} \\ a_6 &= \frac{-(\alpha^3(-8+7\alpha^2))}{3360} & a_7 &= \frac{-(\alpha^2(135+168\alpha^2-128\alpha^4)\sqrt{\pi})}{393216} \end{aligned} \tag{36}$$

for $m = 5$:

$$\begin{aligned} a_2 &= \frac{-\alpha}{12\sqrt{\pi}} & a_3 &= \frac{\alpha^2}{48} \\ a_4 &= \frac{-\alpha^3}{72\sqrt{\pi}} & a_5 &= \frac{\alpha^2(-2+\alpha^2)}{384} \\ a_6 &= \frac{-(\alpha^3(-24+7\alpha^2))}{5040\sqrt{\pi}} & a_7 &= \frac{-9\alpha^4+2\alpha^6}{9216} \end{aligned} \tag{37}$$

for $m = 6$:

$$\begin{aligned} a_2 &= \frac{-\alpha}{64} & a_3 &= \frac{\alpha^2\sqrt{\pi}}{256} \\ a_4 &= -\frac{\alpha^3}{384} & a_5 &= -\frac{\alpha^2(15-4\alpha^2)\sqrt{\pi}}{8192} \\ a_6 &= \frac{-(\alpha^3(-20+3\alpha^2))}{11520} & a_7 &= \frac{\alpha^2(945-1160\alpha^2+128\alpha^4)\sqrt{\pi}}{3145728} \end{aligned} \tag{38}$$

and for $m = 7$:

$$a_2 = \frac{-\alpha}{120\sqrt{\pi}} \qquad a_3 = \frac{\alpha^2}{480}$$
$$a_4 = \frac{-\alpha^3}{720\sqrt{\pi}} \qquad a_5 = \frac{\alpha^2(-6+\alpha^2)}{3840} \tag{39}$$
$$a_6 = \frac{-(\alpha^3(-76+7\alpha^2))}{50\,400\sqrt{\pi}} \qquad a_7 = \frac{\alpha^2(27-15\alpha^2+\alpha^4)}{46\,080}.$$

4. Calculation of the heat kernel asymptotics

The information on the general structure of the heat kernel asymptotic obtained in section 2 can be summarized in the following lemma.

Lemma 1.

(1) *Let $N^\nu(f) = f_{;m\ldots m}$ be the νth normal covariant derivative. There exist invariant local formulae $a_{n,\nu}(y, D)$ so that*

$$a_n(f, D) = \{a_n(f, D_0; x)\}[M] + \left\{ \sum_{0\leqslant\nu\leqslant n-1} N^\nu(f) a_{n,\nu}(y, D) \right\}[\Sigma]. \tag{40}$$

(2) *If we expand $a_{n,\nu}$ with respect to a Weyl basis, the coefficients only depend on the dimension m through a normalizing constant.*

(3) *Consider a transformation which changes the sign before the mth components of all vector and tensor fields and reverses the sign of the extrinsic curvature L_{ab}. Under this transformation $a_{n,\nu} \to (-1)^\nu a_{n,\nu}$.*

(4) *In the linear order of V*

$$a_n(f, D) = \{V(z) \frac{\delta}{\delta E(z)} a_n(f, D_0)\}[\Sigma]. \tag{41}$$

Proof. Assertion (1) is now evident. Volume terms $\{a_n(f, D_0; x)\}[M]$ are given in the appendix B. One can also observe that coefficients before monomials constructed from the geometric invariants depend on the dimension m only through the factor $(4\pi)^{-m/2}$. A more simple way to prove assertion (2) is to consider the product spaces $M = S^1 \times M_1$ and $\Sigma = S^1 \times \Sigma^1$, exactly repeating the corresponding proof for manifolds with boundaries [20]. Assertion (3) follows from the fact that we can repeat all the calculations in section 2 with the replacement $x^m \to -x^m$. The last assertion of lemma 1 is just a trivial generalization of equation (16) for non-unit smearing function f. Indeed, it is sufficient to represent the variation on the rhs of (41) as

$$\frac{\delta}{\delta E(z)} K_0(t) = \int_{\mathcal{M}} \mathrm{d}x \int_0^t \mathrm{d}s\, f(x) K_0(z, x; t-s) K_0(x, z; s). \tag{42}$$

Assertion (4) is now evident.

Now we can determine several first heat kernel coefficients up to a few, as yet undetermined, constants. □

Lemma 2. *There exist universal constants $c_{3,1}, \ldots, c_{5,10}$, such that*

$$
\begin{aligned}
a_0(f,D) &= a_0(f,D_0)\\
a_1(f,D) &= 0\\
a_2(f,D) &= a_2(f,D_0) + (4\pi)^{-m/2}\{fV\}[\Sigma]\\
a_3(f,D) &= (4\pi)^{-(m-1)/2}\{c_{3,1} fV^2\}[\Sigma]\\
a_4(f,D) &= a_4(f,D_0) + (4\pi)^{-m/2}\{c_{4,1} fV^3 + \tfrac{1}{6} f\tau V + fEV\\
&\quad + \tfrac{1}{6} fV_{:aa} - \tfrac{1}{6} f_{;m} V L_{aa} + \tfrac{1}{6} f_{;mm} V\}[\Sigma]\\
a_5(f,D) &= (4\pi)^{-(m-1)/2}\{c_{5,1} fV^4 + c_{5,2} f\tau V^2 + c_{5,3}\rho_{mm} V^2\\
&\quad + c_{5,4} fV^2 E + c_{5,5} fV^2 L_{aa} L_{bb} + c_{5,6} fV^2 L_{ab} L_{ab} + c_{5,7} fV_{:aa} V\\
&\quad + c_{5,8} fV_{:a} V_{:a} + c_{5,9} f_{;m} V^2 L_{aa} + c_{5,10} f_{;mm} V^2\}[\Sigma].
\end{aligned}
\tag{43}
$$

Proof. According to lemma 1 (1) and (2), any coefficient a_n contains all local invariants of appropriate dimension. Some of the invariants, such as, e.g., fVL_{aa}, $f_{;m}V$ etc, are ruled out by lemma 1 (3). All terms linear in V are determined by lemma 1 (4). □

Lemma 3. $c_{3,1} = \frac{1}{8}$, $c_{4,1} = \frac{1}{6}$, $c_{5,1} = \frac{1}{64}$, $c_{5,4} = \frac{1}{8}$, $c_{5,5} = -\frac{1}{256}$, $c_{5,6} = \frac{1}{128}$.

Proof. The coefficients $c_{3,1}$, $c_{4,1}$, $c_{5,1}$, $c_{5,5}$ and $c_{5,6}$ are easily calculated using the example of the δ potential on the sphere of the previous section. To calculate the coefficient $c_{5,4}$, consider the case when $E = e\mathbf{1}$ is a constant proportional to the unit matrix. In this case $K(f;t) = K(f;t)|_{E=0}\exp(te)$. This immediately gives $c_{5,4} = c_{3,1} = \frac{1}{8}$. □

Several more universal constants can be calculated by a reduction to Dirichlet and Neumann boundary value problems. All necessary definitions and explicit expressions for the heat kernel coefficient for that problem can be found in appendix B.

Lemma 4. *(1) Let $M = \Sigma \times [-a, a]$. Let $\nabla_m = \partial_m$ and let all geometric invariants and the smearing function f be symmetric under $x^m \to -x^m$. We suppose that f and a sufficient number of its derivatives vanish at $x^m = \pm a$. Then $a_n(f,D) = a_n(f,D_0,\mathcal{B}^-) + a_n(f,D_0,\mathcal{B}^+)$ where the heat kernel coefficients on the rhs are calculated on $\Sigma \times [0,a]$, and $S = \frac{1}{2}V$.*

Proof. Since reflection of the mth coordinate commutes with D one can subdivide the spectral resolution in the two sets, $(\lambda_\pm^N, \phi_\pm^N)$, with normalized eigenfunctions $\phi_\pm^N(-x^m) = \pm\phi_\pm^N(x^m)$. Then the heat kernel becomes

$$K(f;t) = K_-(f;t) + K_+(f;t) \tag{44}$$

where

$$
\begin{aligned}
K_\pm(f;t) &= \int_M \mathrm{d}x\, f(x) \sum_N \exp(-t\lambda_\pm)\phi_\pm(x)^2\\
&= \int_0^a \mathrm{d}x^m \int_\Sigma \mathrm{d}z\, f(x^m,z) \sum_N \exp(-t\lambda_\pm)(\sqrt{2}\phi_\pm(x^m,z))^2.
\end{aligned}
\tag{45}
$$

Now we observe that $\sqrt{2}\phi_\pm$ are normalized eigenfunctions of the operator D_0 on $\Sigma \times [0,a]$ satisfying Dirichlet and Neumann boundary conditions

$$\phi_-|_{x^m=0} = 0 \qquad (\nabla_m + \tfrac{1}{2}V)\phi_+|_{x^m=0} = 0. \tag{46}$$

The assertion of lemma 4 follows immediately. □

Under the conditions of lemma 4, L_{ab}, ρ_{mm} and $f_{;m}$ vanish identically. We can only calculate the coefficients of $f\tau V^2$, $fV_{:aa}V$, $fV_{:a}V_{:a}$ and $f_{;mm}V^2$.

Corollary. $c_{5,2} = \frac{1}{48}$, $c_{5,7} = \frac{1}{24}$, $c_{5,8} = \frac{5}{192}$, $c_{5,10} = \frac{1}{64}$.

The rest of the universal constants can be calculated by using the conformal properties of the heat kernel which are exactly the same as for the usual boundary value problem [20].

Lemma 5. *If* $D(\epsilon) = \mathrm{e}^{-2f\epsilon}D$, *then* $\frac{\mathrm{d}}{\mathrm{d}\epsilon}|_{\epsilon=0}a_n(1, D) = (m-n)a_n(f, D)$.

Under the conformal transformation the metric g acquires a multiplier $\mathrm{e}^{2f\epsilon}$. V is transformed to $\mathrm{e}^{-f\epsilon}V$. Basic geometric quantities transform as [20]

$$\begin{aligned}
&\left(\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}\Gamma\right)^k_{ij} = \delta_{ik}f_{;j} + \delta_{jk}f_{;i} - \delta_{ij}f_{;k}\\
&\left(\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}L\right)_{ab} = -\delta_{ab}f_{;m} - fL_{ab}\\
&\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}(E) = -2fE + \frac{1}{2}(m-2)f_{;ii}\\
&\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}(\tau) = -2f\tau + 2(1-m)f_{;ii}\\
&\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}(\rho_{mm}) = -2f\rho_{mm} - f_{;aa} + (1-m)f_{;mm}
\end{aligned} \tag{47}$$

where Γ is the Christoffel connection. We need the following conformal relations:

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}V^2\tau = -4fV^2\tau + 2(1-m)[f_{;mm}V^2 + 2f(V_{:aa}V + V_{:a}V_{:a}) - L_{:aa}f_{;m}V^2]\\
&\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}V^2\rho_{mm} = -4V^2\rho_{mm}f - 2f(V_{:aa}V + V_{:a}V_{:a}) + L_{aa}Vf_{;m} + (1-m)V^2f_{;mm}\\
&\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}V^2E = -4V^2Ef + (m-2)f(V_{:aa}V + V_{:a}V_{:a})\\
&\qquad\qquad -\tfrac{1}{2}(m-2)L_{aa}f_{;m}V^2 + \tfrac{1}{2}(m-2)f_{;mm}V^2\\
&\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}V^2L^2_{aa} = -4V^2L^2_{aa}f - 2(m-1)V^2L_{aa}f_{;m}\\
&\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}V^2L_{ab}L_{ab} = -4V^2L_{ab}L_{ab}f - 2V^2L_{aa}f_{;m}\\
&\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}V_{:aa}V = -4V_{:aa}Vf - (m-3)(V_{:aa}Vf + V_{:a}V_{:a}f)\\
&\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}V_{:a}V_{:a} = -4V_{:a}V_{:a}f + 2(V_{:aa}Vf + V_{:a}V_{:a}f).
\end{aligned} \tag{48}$$

To obtain relation (48) we used integration by parts. Let $n = 5$. By collecting the terms with $V_{:aa}Vf$ and $V^2L_{:aa}f_{;m}$ we obtain

$$\begin{aligned}
&0 = 4(1-m)c_{5,2} - 2c_{5,3} + (m-2)c_{5,4} - (m-3)c_{5,7} + 2c_{5,8}\\
&0 = -2(1-m)c_{5,2} + c_{5,3} - \tfrac{1}{2}(m-2)c_{5,4} - 2(m-1)c_{5,5} - 2c_{5,6} - (m-5)c_{5,9}.
\end{aligned}$$

Solving these equation one obtains $c_{5,3} = \frac{1}{192}$ and $c_{5,9} = -\frac{5}{384}$. Below, for the convenience of the reader, we list all the universal constants of lemma 2:

$$\begin{array}{lllll} c_{3,1} = \frac{1}{8} & c_{4,1} = \frac{1}{6} & c_{5,1} = \frac{1}{64} & c_{5,2} = \frac{1}{48} & c_{5,3} = \frac{1}{192} \\ c_{5,4} = \frac{1}{8} & c_{5,5} = -\frac{1}{256} & c_{5,6} = \frac{1}{128} & c_{5,7} = \frac{1}{24} & c_{5,8} = \frac{5}{192} \\ c_{5,9} = -\frac{5}{384} & c_{5,10} = \frac{1}{64}. & & & \end{array} \tag{49}$$

5. Conclusions

In this paper we have studied the heat kernel expansion for a Laplace-type operator in the presence of semitransparent boundaries. We have determined the general form of the asymptotic expansion. Namely, we proved the validity of the asymptotic series (11). We have explicitly calculated several of the first terms of the expansion for the most general operator of Laplace type and arbitrary boundary potential. We believe that this is the most complete study performed in this field so far.

Our methods of deriving the heat kernel coefficients admit extensive cross-checking. Most of the universal constants can be calculated by at least two independent methods. If needed, one can calculate the higher coefficients as well. As possible generalizations, we can suggest the δ' potentials or even general four-parameter family on matching conditions [1] on the hypersurface Σ. Another possible development of the present results could be the renormalization of quantum field theory in the presence of singular interactions [21]. We believe that semitransparent boundaries provide a more adequate framework for the renormalization than the 'abrupt' boundary conditions of Dirichlet or Neumann type. For most recent work on renormalization with singular potentials, see [17].

Acknowledgments

We are grateful to Klaus Kirsten for fruitful discussions. DV thanks the Alexander von Humboldt foundation and RFBR, grant 97-01-01186. He is also grateful to S Randjbar-Daemi for kind hospitality at the Abdus Salam ICTP where this work was completed.

Appendix A

Some of the first non-zero coefficients, $X_{n,i}$, appearing in (31) read:

$$\begin{array}{llll} X_{1,1} = \dfrac{\alpha}{2} & X_{2,2} = \dfrac{-\alpha^2}{8} & X_{3,3} = \dfrac{\alpha}{16} + \dfrac{\alpha^3}{24} & X_{3,5} = \dfrac{-3\alpha}{8} \\ X_{3,7} = \dfrac{5\alpha}{16} & X_{4,4} = \dfrac{-\alpha^2}{32} - \dfrac{\alpha^4}{64} & X_{4,6} = \dfrac{3\alpha^2}{16} & X_{4,8} = \dfrac{-5\alpha^2}{32} \\ X_{5,5} = \dfrac{27\alpha}{256} + \dfrac{\alpha^3}{64} + \dfrac{\alpha^5}{160} & X_{5,7} = \dfrac{-145\alpha}{64} - \dfrac{3\alpha^3}{32} & & \\ X_{5,9} = \dfrac{1085\alpha}{128} + \dfrac{5\alpha^3}{64} & X_{5,11} = \dfrac{-693\alpha}{64} & X_{5,13} = \dfrac{1155\alpha}{256}. & \end{array}$$

The zeta functions defined in equation (33) are

$$\zeta(2, n) = 2\zeta_{\mathrm{R}}(2s + n)$$
$$\zeta(3, n) = 2\zeta_{\mathrm{H}}(2s + n - 1; \tfrac{1}{2})$$
$$\zeta(4, n) = \zeta_{\mathrm{R}}(2s + n - 2)$$

$$\zeta(5,n) = \frac{2}{3!}(\zeta_{\rm H}(2s+n-3;\tfrac{1}{2}) - \tfrac{1}{4}\zeta_{\rm H}(2s+n-1;\tfrac{1}{2}))$$
$$\zeta(6,n) = \frac{2}{4!}(\zeta_{\rm R}(2s+n-4) - \zeta_{\rm R}(2s+n-2))$$
$$\zeta(7,n) = \frac{2}{5!}(\zeta_{\rm H}(2s+n-5;\tfrac{1}{2}) - \tfrac{5}{2}\zeta_{\rm H}(2s+n-3;\tfrac{1}{2}) + \tfrac{9}{16}\zeta_{\rm H}(2s+n-1;\tfrac{1}{2}))$$

where $\zeta_{\rm R}$ and $\zeta_{\rm H}$ are the Riemann and Hurwitz zeta functions, correspondingly.

Appendix B

In this appendix we give expressions for the heat kernel coefficients for the Dirichlet and Neumann boundary value problems. Let M be a smooth compact Riemannian manifold with smooth boundary ∂M. Let S be an endomorphism on $\mathcal{V}_{\partial M}$ and let $\phi_{;m}$ be a covariant derivative of ϕ with respect to inward unit normal. We define the modified Neumann boundary operator $\mathcal{B}^+$ and the Dirichlet boundary operator $\mathcal{B}^-$ by

$$\mathcal{B}^+\phi := (\phi_{;m} + S\phi)|_{\partial M} \qquad \mathcal{B}^-\phi := \phi|_{\partial M}. \tag{50}$$

We set $S = 0$ for the Dirichlet boundary conditions to ensure uniform notation.

We only need the case of a totally geodesic boundary ($L_{ab} = 0$). We drop certain boundary invariants which vanish under the conditions of lemma 4. One of the first heat kernel coefficients are [14, 20, 22]

$$\begin{aligned}
a_0(f,D,\mathcal{B}^\pm) &= (4\pi)^{-m/2}\,\mathrm{Tr}(f)[M] \\
a_1(f,D,\mathcal{B}^\pm) &= \pm\tfrac{1}{4}(4\pi)^{-(m-1)/2}\,\mathrm{Tr}(f)[\partial M] \\
a_2(f,D,\mathcal{B}^\pm) &= (4\pi)^{-m/2}\tfrac{1}{6}\,\mathrm{Tr}\{(6FE + F\tau)[M] + 12fS[\partial M]\} \\
a_3(f,D,\mathcal{B}^\pm) &= \pm\tfrac{1}{384}(4\pi)^{-(m-1)/2}\,\mathrm{Tr}\{f(96E + 16\tau + 192S^2) + 24F_{;mm}\}[\partial M] \\
a_4(f,D,\mathcal{B}^\pm) &= (4\pi)^{-m/2}\tfrac{1}{360}\,\mathrm{Tr}(f(60E_{;kk} + 60\tau E + 180E^2 + 30\Omega^2 + 12\tau_{;kk} \\
&\quad +5\tau^2 - 2\rho^2 + 2R^2)[M] + (f(720SE + 120S\tau + 480S^3 \\
&\quad +120S_{:aa}) + 120f_{;mm}S)[\partial M]) \\
a_5(f,D,\mathcal{B}^\pm) &= \pm\tfrac{1}{5760}(4\pi)^{-(m-1)/2}\,\mathrm{Tr}\{f(360E_{;mm} + 1440E_{;m}S + 720E^2 \\
&\quad +2880ES^2 + 1440S^4 + 240E_{:aa} + 240\tau E + 120\Omega_{ab}\Omega_{ab} \\
&\quad +20\tau^2 - 8\rho^2 + 8R^2 + 480\tau S^2 + 960S_{:aa}S + 600S_{:a}S_{:a}) \\
&\quad +f_{;mm}(360E + 360S^2 + 60\tau) + 45f_{;mmmm}\}[\partial M].
\end{aligned} \tag{51}$$

On a manifold without a boundary one should keep volume contributions only.

References

[1] Albeverio S, Gesztesy F, Hoegh-Krohn R and Holden H 1988 *Solvable Models in Quantum Mechanics* (New York: Springer)

[2] Berezin F A and Faddeev L D 1961 *Sov. Math. Dokl.* **2** 372

[3] Vilenkin A and Shellard E P S 1994 *Cosmic Strings and Other Topological Defects* (Cambridge: Cambridge University Press)

[4] Frolov V P and Fursaev D V 1998 *Class. Quantum Grav.* **15** 2041

[5] Apps J S and Dowker J S 1998 *Class. Quantum Grav.* **15** 1121

[6] Bordag M, Hennig D and Robaschik D 1992 *J. Phys. A: Math. Gen.* **25** 4483–98

[7] Jaekel M-T and Reynaud S 1992 *Phys. Lett.* A **167** 227–32

[8] Actor A A 1995 *Phys. Rev.* D **52** 3581–90

[9] Gilkey P B 1994 *Invariance Theory, the Heat Equation and the Atiyah–Singer Index Theorem* (Boca Raton, FL: Chemical Rubber Company)

[10] Scandurra M 1999 *J. Phys. A: Math. Gen.* **32** 5679
(Scandurra M 1998 The ground state energy of a massive scalar field in the background of a semitransparent spherical shell *Preprint* hep-th/9811164)
[11] Bordag M and Kirsten K 1998 *Phys. Rev.* D **60** 105019
(Bordag M and Kirsten K 1998 The ground state energy of a spinor field in the background of a finite radius flux tube *Preprint* hep-th/9812060)
[12] Schwinger J, DeRaad L L and Milton K A 1978 *Ann. Phys., NY* **115** 1
[13] Bordag M, Kirsten K and Vassilevich D V 1999 *Phys. Rev.* D **59** 085011
[14] Branson T P, Gilkey P B and Vassilevich D V 1997 *Boll. Unione Mat. Ital.* B **11** Suppl. Fasc. 2 39, hep-th/9504029
[15] Grubb G 1986 *Functional Calculus of Pseudo Differential Boundary Problems (Progress in Mathematics vol 65)* (Boston, MA: Birkhäuser)
[16] Albeverio S, Brzezniak Z and Dabrowski L 1994 *J. Phys. A: Math. Gen.* **27** 4933
[17] Solodukhin S N 1999 *Nucl. Phys.* B **539** 403
[18] Gaveau B and Schulman L S 1986 *J. Phys. A: Math. Gen.* **19** 1833
[19] Bordag M, Kirsten K and Elizalde E 1996 *J. Math. Phys.* **37** 895
[20] Branson T P and Gilkey P B 1990 *Commun. Partial Diff. Eqns* **15** 245
[21] Symanzik K 1981 *Nucl. Phys.* B **190** 1
[22] Kirsten K 1998 *Class. Quantum Grav.* **15** L5