Heat Kernel Asymptotics of Zaremba Boundary Value Problem

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The Zaremba boundary-value problem is a boundary value problem for Laplace-type second-order partial differential operators acting on smooth sections of a vector bundle over a smooth compact Riemannian manifold with smooth boundary but with non-smooth (singular) boundary conditions, which include Dirichlet conditions on one part of the boundary and Neumann ones on another part of the boundary. We study the heat kernel asymptotics of Zaremba boundary value problem. The construction of the global parametrix of the heat equation is described in detail and the leading parametrix is computed explicitly. Some of the first non-trivial coefficients of the heat kernel asymptotic expansion are computed explicitly.
1 Introduction

The heat kernel of elliptic partial differential operators acting on sections of vector bundles over compact manifolds proved to be of great importance in mathematical physics. In particular, the main objects of interest in quantum field theory and statistical physics, such as the effective action, the partition function, Green functions, and correlation functions, are described by the functional determinants and the resolvent of differential operators, which can be expressed in terms of the heat kernel. The most important operators appearing in physics and geometry are the second order partial differential operators of Laplace type; such operators are characterized by a scalar leading symbol (even if acting on sections of vector bundles). Within the smooth category this problem has been studied extensively during last years (see, for example, [30, 10]; for reviews see [4, 3] and references therein). In the case of smooth compact manifolds without boundary the problem of calculation of heat kernel asymptotics reduces to a purely computational (algebraic) one for which various powerful algorithms have been developed [1, 43]; this problem is now well understood. In the case of smooth compact manifolds with a smooth boundary and smooth boundary conditions the complexity of the problem depends significantly on the type of the boundary conditions. The classical smooth boundary problems (Dirichlet, Neumann, or a mixed combination of those on vector bundles) are the most extensively studied ones (see [12, 13, 34, 2] and the references therein). A more general scheme, so called oblique (or Grubb-Gilkey-Smith) boundary value problem [31, 29, 28], which includes tangential (oblique) derivatives along the boundary, has been studied in [7, 8, 6, 22, 23, 24]. In this case the problem is not automatically elliptic; there is a certain strong ellipticity condition on the leading symbol of the boundary operator. This problem is much more difficult to handle, the main reason being that the heat kernel asymptotics are no longer polynomial in the jets of the symbols of the differential operator and the boundary operator. Another class of boundary value problems are characterized by essentially non-local boundary conditions, for example, the spectral or Atiyah-Patodi-Singer boundary conditions [30, 32, 11, 38].

All the above described boundary value problems were smooth. A more general (and much more complicated) setting, so called singular boundary value problem, arises when either the symbol of the differential operator or the symbol of the boundary operator (or the boundary itself) are not smooth. In this paper we study a singular boundary value problem for a second order par-
tial differential operator of Laplace type when the operator itself has smooth coefficients but the boundary operator is not smooth. For the case when the manifold as well as the boundary are smooth, but the boundary operator jumps from Dirichlet to Neumann on the boundary, is known in the literature as Zaremba problem. Such problems often arise in applied mathematics and engineering and there are some exact results available for special cases (two or three dimensions, specific geometry, etc.) [12 25]. Zaremba problem belongs to a much wider class of singular boundary value problems, i.e. manifolds with singularities (corners, edges, cones etc.). There is a large body of literature on this subject where the problem is studied from an abstract function-analytical point of view [20, 17, 18, 10, 2, 5, 11, 97, 33, 33, 27]. However, the study of heat kernel asymptotics of Zaremba type problems is quite new, and there are only some preliminary results in this area [3, 21, 20]. Moreover, compared to the smooth category the needed machinery is still underdeveloped. We would like to stress that we are interested not only in the asymptotics of the trace of the heat kernel, i.e. the integrated heat kernel diagonal, but also in the local asymptotic expansion of the off-diagonal heat kernel.

This paper is organized as follows. In the sect. 2 a formal description of the Zaremba problem is given. In the sect. 3 the general form of the heat kernel asymptotic expansion is described. In sect. 4 the construction of the global parametrix to the heat equation is described. In sect. 5 the first non-trivial heat kernel coefficients are computed explicitly. In conclusion we summarize (and discuss) the results and outline some future problems.

2 General Setup

2.1 Laplace Type Operators

Let \((M, g)\) be a smooth compact Riemannian manifold of dimension \(m\) with a boundary \(\partial M\), equipped with a positive definite Riemannian metric \(g\). Let \(V\) be a vector bundle over \(M\), \(V^*\) be its dual, and \(\text{End}(V) \cong V \otimes V^*\) be the corresponding bundle of endomorphisms. Given any vector bundle \(V\), we denote by \(C^\infty(V)\) its space of smooth sections. We assume that the vector bundle \(V\) is equipped with a Hermitian metric. This naturally identifies the dual vector bundle \(V^*\) with \(V\), and defines a natural \(L^2\) inner product and the \(L^2\)-trace using the invariant Riemannian measure \(d\text{vol}_g\) on the manifold.
The completion of $C^\infty(V)$ in this norm defines the Hilbert space $L^2(V)$ of square integrable sections.

We denote by $TM$ and $T^*M$ the tangent and cotangent bundles of $M$. Let a connection, $\nabla^V : C^\infty(V) \to C^\infty(TM \otimes V)$, on the vector bundle $V$ be given, which we assume to be compatible with the Hermitian metric on the vector bundle $V$. The connection is given its unique natural extension to bundles in the tensor algebra over $V$ and $V^*$. In fact, using the Levi-Civita connection $\nabla^{LC}$ of the metric $g$ together with $\nabla^V$, we naturally obtain connections on all bundles in the tensor algebra over $V$, $V^*$, $TM$ and $T^*M$; the resulting connection will usually be denoted just by $\nabla$. It is usually clear which bundle’s connection is being referred to, from the nature of the section being acted upon. We also adopt the Einstein convention and sum over repeated indices. With our notation, Greek indices, $\mu, \nu, \ldots$, label the local coordinates on $M$ and range from 1 through $m$, lower case Latin indices from the middle of the alphabet, $i, j, k, l, \ldots$, label the local coordinates on $\partial M$ (codimension one manifold) and range from 2 through $m$, and lower case Latin indices from the beginning of the alphabet, $a, b, c, d, \ldots$, label the local coordinates on a codimension two manifold $\Sigma_0 \subset \partial M$ that will be described later and range over $3, \ldots, m$. Further, we will denote by $\tilde{g}$ the induced metric on the submanifolds (of the codimension one or two) and by $\tilde{\nabla}$ the Levi-Civita connection of the induced metric. We should stress from the beginning that we slightly abuse the notation by using the same symbols for all submanifolds (of codimension one and two). This should not cause any misunderstanding since it is always clear from the context what is meant.

Let $\nabla^*$ be the formal adjoint of the covariant derivative defined using the Riemannian metric and the Hermitian structure on $V$ and let $Q \in C^\infty(\text{End}(V))$ be a smooth Hermitian section of the endomorphism bundle $\text{End}(V)$. The Laplace type operator $F : C^\infty(V) \to C^\infty(V)$ is a partial differential operator of the form

$$F = \nabla^* \nabla + Q = -g^{\mu\nu} \nabla_\mu \nabla_\nu + Q.$$  \hspace{1cm} (1)

Alternatively, the Laplace type operators are second-order partial differential operators with positive definite scalar leading symbol of the form $\sigma_L(F; x, \xi) = I|\xi|^2 = I g^{\mu\nu}(x) \xi_\mu \xi_\nu$. Hereafter $I$ denotes the identity endomorphism of the vector bundle $V$. We will often omit it whenever it does not cause any misunderstanding. Any second order operator with a scalar leading symbol can be put in the form $|I|$ by choosing the Riemannian metric $g$, the connection $\nabla^V$ on the vector bundle $V$ and the endomorphism $Q$. 

$M$. The completion of $C^\infty(V)$ in this norm defines the Hilbert space $L^2(V)$ of square integrable sections.
2.2 Boundary Conditions

In the case of manifolds with boundary, one has to impose some boundary conditions in order to make a (formally self-adjoint) differential operator self-adjoint (at least symmetric) and elliptic. Let $N$ be the inward-pointing unit normal vector field to the boundary and let $W = V|_{\partial M}$ be the restriction of the vector bundle $V$ to the boundary $\partial M$. We define the boundary data map

$$\psi : C^\infty(V) \to L^2(W \oplus W)$$

by

$$\psi(\varphi) = \begin{pmatrix} \varphi|_{\partial M} \\ \nabla_N \varphi|_{\partial M} \end{pmatrix}.$$  \hspace{1cm} (2)

The boundary conditions then read

$$B \psi(\varphi) = 0,$$

where $B : L^2(W \oplus W) \to L^2(W \oplus W)$ is the boundary operator, which will be specified later. If the operator $B$ is a tangential differential operator (possibly of order zero), then the boundary conditions are local. Otherwise, for example, when $B$ is a pseudo-differential operator, the boundary conditions are non-local.

To define the boundary operator one needs a self-adjoint orthogonal projector $\Pi$ that splits the space $L^2(W)$ in two orthogonal subspaces

$$L^2(W) = L^2_\| (W) \oplus L^2_\perp (W),$$  \hspace{1cm} (4)

where

$$L^2_\| (W) = \Pi L^2(W), \hspace{1cm} \text{and} \hspace{1cm} L^2_\perp = (\text{Id} - \Pi) L^2(W),$$

and a self-adjoint operator $\Lambda : L^2(W) \to L^2(W)$, such that $\Lambda L^2_\| (W) = \{0\}$, i.e. $\Pi \Lambda = \Lambda \Pi = 0$. Hereafter $\text{Id}$ denotes the identity operator. The boundary operator is then defined by

$$B = \begin{pmatrix} \Pi & 0 \\ \Lambda & \text{Id} - \Pi \end{pmatrix},$$  \hspace{1cm} (6)

which is equivalent to the following boundary conditions

$$\Pi \left( \varphi\Big|_{\partial M} \right) = 0,$$

$$\left( \text{Id} - \Pi \right) \left( \nabla_N \varphi\Big|_{\partial M} \right) + \Lambda \left( \varphi\Big|_{\partial M} \right) = 0,$$  \hspace{1cm} (8)
It is easy to see that the boundary operator $B$ and the operator 

$$K = \text{Id} - B = \begin{pmatrix} \text{Id} - \Pi & 0 \\ -\Lambda & \Pi \end{pmatrix},$$

are complimentary projectors on $L^2(W \oplus W)$, i.e.

$$B^2 = B \quad K^2 = K, \quad BK = KB = 0.$$  \hspace{1cm} (10)

Hence, a section that satisfies the boundary conditions can be parametrized by $\chi(\varphi) = u(\varphi) \oplus v(\varphi) \in L^2(W \oplus W)$, $u(\varphi) \in L^2_{\perp}$, $v(\varphi) \in L^2_{||}$, so that

$$\psi(\varphi) = K\chi(\varphi) = \begin{pmatrix} u(\varphi) \\ -\Lambda u(\varphi) + v(\varphi) \end{pmatrix}. \hspace{1cm} (11)$$

It is not difficult to see that the boundary operator $B$ incorporates all standard types of boundary conditions. Indeed, by choosing $\Pi = I$ and $\Lambda = 0$ one gets the Dirichlet boundary conditions, by choosing $\Pi = 0$, $\Lambda = I$ one gets the Neumann boundary conditions. More generally, the choice $\Pi, \Lambda \in C^\infty(\text{End}(W))$, so that $\Lambda\Pi = \Pi\Lambda = 0$, corresponds to the mixed boundary conditions.

**Remark 1** The boundary $\partial M$ could be, in general, a disconnected manifold consisting of a finite number of disjoint connected parts, $\partial M = \bigcup_{i=1}^n \Sigma_i$, with each $\Sigma_i$ being compact connected manifold without boundary, $\partial\Sigma_i = \emptyset$ and $\Sigma_i \cap \Sigma_j = \emptyset$ if $i \neq j$. Thus one can impose different boundary conditions on different connected parts of the boundary $\Sigma_i$. This means that the full boundary operator decomposes $B = B_1 \oplus \cdots \oplus B_n$, with $B_i$ being different boundary operators acting on different bundles.

We always assume the manifold $M$ itself and the coefficients of the operator $F$ to be smooth in the interior of $M$. If, in addition, the boundary $\partial M$ is smooth, and the boundary operator $B$ is a differential operator with smooth coefficients, then $(F, B)$ is called smooth local boundary value problem.

In this paper we are interested in a different class of boundary conditions. Namely, we do not assume the boundary operator to be smooth. Instead, we will study the case when it has discontinuous coefficients. Such problems are often called mixed boundary conditions; to avoid misunderstanding we will not use this terminology. We impose different boundary conditions.
on connected parts of the boundary, which makes the boundary value problem discontinuous. Roughly speaking, one has a decomposition of a smooth boundary in some parts where different types of the boundary conditions are imposed, i.e. Dirichlet or Neumann. The boundary operator is then discontinuous at the intersection of these parts. The boundary value problems of this type are called Zaremba problem in the literature [14, 15] (see also [12, 23, 5, 21, 20]).

In this paper we consider the simplest case when there are just two components. We assume that the boundary of the manifold \( \partial M \) is decomposed as the disjoint union

\[
\partial M = \Sigma_1 \cup \Sigma_2 \cup \Sigma_0, \tag{12}
\]

where \( \Sigma_1 \) and \( \Sigma_2 \) are smooth compact submanifolds of dimension \((m - 1)\) (codimension 1 submanifolds), with the same boundary \( \Sigma_0 = \partial \Sigma_1 = \partial \Sigma_2 \), that is a smooth compact submanifold of dimension \((m - 2)\) (codimension 2 submanifold) without boundary, i.e. \( \partial \Sigma_0 = \emptyset \). Let us stress here that when viewed as sets both \( \Sigma_1 \) and \( \Sigma_2 \) are considered to be disjoint open sets, i.e. \( \Sigma_1 \cap \Sigma_2 = \emptyset \).

Let \( \chi_i : \partial M \rightarrow \mathbb{R}, (i = 0, 1, 2) \), be the characteristic functions of the sets \( \Sigma_i \), \( \chi_i(\hat{x}) = 1 \) if \( \hat{x} \in \Sigma_i \) and \( \chi_i(\hat{x}) = 0 \) if \( \hat{x} \not\in \Sigma_i \). Obviously, \( \chi_1(\hat{x}) + \chi_2(\hat{x}) + \chi_0(\hat{x}) = 1 \) for any \( \hat{x} \in \partial M \). Let \( \pi_i : L^2(W) \rightarrow L^2(W), (i = 0, 1, 2) \), be the trivial projections of sections, \( \psi \), of a vector bundle \( W \) to \( \Sigma_i \) defined by \( (\pi_i \psi)(\hat{x}) = \chi_i(\hat{x}) \psi(\hat{x}) \), i.e. \( (\pi_i \psi)(\hat{x}) = \psi(\hat{x}) \) if \( \hat{x} \in \Sigma_i \) and \( (\pi_i \psi)(\hat{x}) = 0 \) if \( \hat{x} \not\in \Sigma_i \). In other words \( \pi_1 \) maps smooth sections of the bundle \( W \) to their restriction to \( \Sigma_1 \), extending them by zero on \( \Sigma_2 \), and similarly for \( \pi_2 \). Obviously, \( \pi_1 + \pi_2 + \pi_0 = \text{Id}, \pi_i^2 = \pi_i, (i = 0, 1, 2) \), and \( \pi_i \pi_j = 0 \) for \( i \neq j \).

Let \( \Lambda \in C^\infty(\text{End}(W)) \) be a smooth Hermitian endomorphism of the vector bundle \( W \). Then the boundary operator of our problem can be written in the form

\[
B = \begin{pmatrix}
\pi_1 & 0 \\
\pi_2 \Lambda \pi_2 & \pi_2
\end{pmatrix}, \tag{13}
\]

The projectors \( \pi_1 \) and \( \pi_2 \) as well as the boundary operator \( B \) are clearly non-smooth (discontinuous) on \( \Sigma_0 \). In other words, we have Dirichlet boundary conditions on \( \Sigma_1 \) and Neumann (Robin) boundary conditions on \( \Sigma_2 \):

\[
\varphi|_{\Sigma_1} = 0, \tag{14}
\]

\[
(\nabla_N + \Lambda)\varphi|_{\Sigma_2} = 0 \tag{15}
\]
Note that the boundary conditions are set only on open subsets $\Sigma_1$ and $\Sigma_2$; the boundary conditions do not say anything about the boundary data on $\Sigma_0$. We will see later that to specify the solution uniquely we also need a further condition which specifies the type of the singularity on $\Sigma_0$.

We will call the boundary value problem $(F, B)$ for a Laplace operator $F$ with the boundary operator $B$ of the form \[1\] Zaremba boundary value problem.

### 2.3 Symmetry

Let us define the antisymmetric bilinear form

\[ I(\varphi_1, \varphi_2) \equiv (F\varphi_1, \varphi_2)_{L^2(V)} - (\varphi_1, F\varphi_2)_{L^2(V)}, \quad (16) \]

for any two smooth sections $\varphi_1, \varphi_2 \in C^\infty(V)$ of the vector bundle $V$. By integrating by parts on $M$ one can easily see that this bilinear form depends only on the boundary data

\[ I(\varphi_1, \varphi_2) = (\psi(\varphi_1), J\psi(\varphi_2))_{L^2(W \oplus W)}, \quad (17) \]

where

\[ J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \quad (18) \]

Therefore, it vanishes on sections of the bundle $V$ with compact support disjoint from the boundary $\partial M$ when the boundary data vanish $\psi(\varphi_1) = \psi(\varphi_2) = 0$. This is a simple consequence of the fact that the operator $F$ is \textit{formally self-adjoint}. A formally self-adjoint operator is \textit{essentially self-adjoint} if its closure is self-adjoint. This means that the operator is such that: i) it is \textit{symmetric} on smooth sections satisfying the boundary conditions, and ii) there exists a unique self-adjoint extension of it. To prove the latter property one has to study the deficiency indices; however, this will not be the subject of primary interest in the present paper. We check only the first property, i.e. that the operator $F$ is symmetric.

By integrating by parts on $\partial M$, it is not difficult to check that the form $I(\varphi_1, \varphi_2)$ does vanish for any $\varphi_1, \varphi_2 \in C^\infty(V)$ satisfying the boundary conditions with the boundary operator \[2\] provided the operator $\Lambda$ is symmetric. Therefore, we immediately obtain that the Zaremba boundary value problem is symmetric.
2.4 Ellipticity

Let $F_0$ be a Laplace type operator with constant coefficients obtained from the operator $F$ by freezing the coefficients at a fixed point $x_0$ in the leading derivative part, i.e. for the Laplace type operator $F_0 = -g^\mu\nu(x_0)\partial_\mu\partial_\nu$. If the point $x_0$ is in the interior of the manifold $M$, we assume the operator $F_0$ to act on the sections of the vector bundle $V$ over $\mathbb{R}^m$. If the point $x_0$ is on the boundary, we assume the operator $F_0$ to act on sections of $V$ over $\mathbb{R}^{m-1} \times \mathbb{R}_+$. If the point $x_0$ is on the boundary, we also define the operator $B_0$ by omitting the non-diagonal part of $B$ and freezing the coefficients of the diagonal part of the boundary operator $B$, i.e. $B_0 = \chi_1(\hat{x}_0) \oplus \chi_2(\hat{x}_0)$. Note that the coefficients of the operator $B_0$ are constant on $\Sigma_1$ and $\Sigma_2$ but are discontinuous on $\Sigma_0$.

The boundary value problem $(F, B)$ is said to be elliptic with respect to $\mathbb{C} \setminus \mathbb{R}_+$ if for any complex number $\lambda \in \mathbb{C} \setminus \mathbb{R}_+$ not lying on the positive real axis the following two conditions are satisfied: i) for any interior point $x_0$ the equation

$$(F_0 - \lambda)\varphi = 0 \quad (19)$$

has a unique non-trivial solution vanishing at infinity, and ii) for any boundary point $\hat{x}_0$ the above equation has a unique non-trivial solution vanishing at infinity and satisfying the boundary conditions

$$B_0\psi(\varphi) = 0. \quad (20)$$

Here non-trivial solution means that it is not identically zero, $\varphi \neq 0$, for $\lambda \neq 0$ and it is not constant, $\varphi \neq \text{const}$, in case $\lambda = 0$.

The question of ellipticity of Zaremba boundary value problem is a subtle one. We will show below that for the freezed problem to have a unique solution one has to impose an additional condition along the codimension two submanifold $\Sigma_0$, which specifies the (singular) behavior of the solution near $\Sigma_0$. Without this condition (which is often imposed implicitly by choosing the most regular solution) the freezed problem has infinitely many acceptable (square integrable) solutions, so that Zaremba problem fails to be elliptic.

3 Heat Kernel

For $t > 0$ the heat semi-group operator $U(t) = \exp(-tF) : L^2(V, M) \to L^2(V, M)$ is well defined. The kernel of this operator, called the heat kernel,
is defined by the equation
\[(\partial_t + F)U(t|x, x') = 0\] (21)
with the initial condition
\[U(0|x, x') = \delta(x, x'),\] (22)
where \(\delta(x, x')\) is the covariant Dirac distribution, the boundary condition
\[B\psi[U(t|x, x')] = 0.\] (23)
and the self-adjointness condition
\[U(t|x, x') = U^*(t|x', x).\] (24)
Hereafter all differential operators as well as the boundary data map act on the first argument of the heat kernel, unless otherwise stated.

Let \(\lambda\) be a complex number with a sufficiently large negative real part, \(\text{Re} \lambda << 0\). The resolvent can then be defined by the Laplace transform
\[G(\lambda) = \int_0^\infty dt e^{t\lambda}U(t),\] (25)
and by analytical continuation elsewhere. The heat kernel can be expressed, in turn, in terms of the resolvent by the inverse Laplace transform
\[U(t) = \frac{1}{2\pi i} \int_{w-i\infty}^{w+i\infty} d\lambda e^{-t\lambda}G(\lambda),\] (26)
where \(w\) is a sufficiently large negative real number, \(w << 0\). As it has been done here, we will sometimes omit the space arguments if it does not cause any confusion.

It is well known \[30\] that the heat kernel \(U(t|x, x')\) is a smooth function near diagonal of \(M \times M\), i.e. for \(x\) close to \(x'\), and has a well defined diagonal value
\[U^{\text{diag}}(t|x) = U(t|x, x),\] (27)
and the functional trace
\[\text{Tr}_{L^2} \exp(-tF) = \int_M \text{tr}_V U^{\text{diag}}(t),\] (28)
where $\text{tr}_V$ is the fiber trace and the integration is defined with the help of the usual Riemannian volume element $d\text{vol}_g$.

It is also well known that in the smooth category the trace of the heat kernel has an asymptotic expansion as $t \to 0^+$ of the form

$$\text{Tr}_{L^2} \exp(-tF) \sim \sum_{k=0}^{\infty} t^{(k-m)/2} A_k.$$  \hspace{1cm} (29)$$

Here $A_k$ are the famous so-called (global) heat-kernel coefficients (sometimes called also Minakshisundaram-Plejel coefficients). They have the following general form \[30\]:

$$A_{2k} = \int_M a^{(0)}_{2k} + \int_{\partial M} a^{(1)}_{2k},$$  \hspace{1cm} (30)$$

$$A_{2k+1} = \int_{\partial M} a^{(1)}_{2k+1},$$  \hspace{1cm} (31)$$

where $a^{(0)}_k$ and $a^{(1)}_k$ are the (local) interior and boundary heat-kernel coefficients. The local interior coefficients $a^{(0)}_k$ are also called HMDS (Hadamard-Minakshisundaram-De Witt-Seeley) coefficients in the literature. Hereafter the integration over the boundary is defined with the help of the usual Riemannian volume element $d\text{vol}_\hat{g}$ on $\partial M$ with the help of the induced metric $\hat{g}$.

The interior coefficients $a^{(0)}_k$ do not depend on the boundary conditions $B$. The even order coefficients $a^{(0)}_{2k}$ are calculated for Laplace-type operators up to $a^{(0)}_8$ \[1, 13\]. The boundary coefficients $a^{(1)}_k$ do depend on both the operator $F$ and the boundary operator $B$. They are far more complicated because in addition to the geometry of the manifold $M$ they depend essentially on the geometry of the boundary $\partial M$. For Laplace-type operators they are known for the usual boundary conditions (Dirichlet, Neumann, or mixed version of them) up to $a^{(1)}_5$ \[12, 13, 34\]. For oblique boundary conditions including tangential derivatives some coefficients were recently computed in \[33, 4, 8, 9, 22, 23\].

However, the boundary value problem considered in the present paper with Zaremba type boundary operator $B$ \[13\] is essentially singular. Even if the manifold $M$, its boundary $\partial M$ and the operator $F$ are all in smooth category, the coefficients of the boundary operator $B$ are discontinuous on
\( \Sigma_0 \), which makes it a \textit{singular problem}. For such problems the asymptotic expansion of the trace of the heat kernel has additional \textit{non-trivial logarithmic terms}\([27, 13]\)

\[
\text{Tr}_{L^2} \exp(-tF_B) \sim \sum_{k=0}^{\infty} t^{(k-m)/2} B_k + \log t \sum_{k=0}^{\infty} t^{k/2} H_k.
\]

(32)

Whereas there are some results concerning the coefficients \( B_k \), almost nothing is known about the coefficients \( H_k \). Since the Zaremba problem is local, or better to say ‘pseudo-local’, all these coefficients have the form

\[
B_{2k} = \int_M b_{2k}^{(0)} + \int_{\Sigma_1} b_{2k}^{(1),1} + \int_{\Sigma_2} b_{2k}^{(1),2} + \int_{\Sigma_0} b_{2k}^{(2)},
\]

(33)

\[
B_{2k+1} = \int_{\Sigma_1} b_{2k+1}^{(1),1} + \int_{\Sigma_2} b_{2k+1}^{(1),2} + \int_{\Sigma_0} b_{2k+1}^{(2)},
\]

(34)

\[
H_k = \int_{\Sigma_0} h_k.
\]

(35)

Here the new feature is the appearance of the integrals over \( \Sigma_0 \), which complicates the problem even more, since the coefficients now depend on the geometry of the imbedding of the codimension 2 submanifold \( \Sigma_0 \) in \( M \) that could be pretty complicated, even if smooth. The asymptotic expansion of the trace of the heat kernel has been studied recently in \([40]\). It has been shown there that the logarithmic terms do not appear, i.e. \( H_k = 0 \) for any \( k \), in the Zaremba type problem considered in the present paper, which confirmed the conjecture of \([5]\).

### 4 Parametrix of the Heat Equation

Let us stress here that we are not going to provide a rigorous construction of the parametrix with all the estimates, which, for a singular boundary-value problem, is a task that would require a separate paper. For such a treatment the reader is referred to the papers \([38, 39, 29, 28, 11, 32]\) for the smooth case and to \([26, 17, 13, 14, 13, 11, 8, 8, 8, 8, 8, 8]\) for the singular case.

Here we shall adhere instead to a pragmatic approach and will describe the construction of the parametrix that can be used to calculate \textit{explicitly} the heat kernel coefficients \( B_k \) as well as \( H_k \).
4.1 Geometrical Framework

First of all, we need to describe properly the geometry of the problem. Let us fix two small positive numbers \( \varepsilon_1, \varepsilon_2 > 0 \). We split the whole manifold in a disjoint union of four different parts:

\[
M = M^{\text{int}} \cup M^{\text{bnd}} = M^{\text{int}} \cup M_1^{\text{bnd}} \cup M_2^{\text{bnd}} \cup M_0^{\text{bnd}}. \tag{36}
\]

Here \( M_0^{\text{bnd}} \) is defined as the set of points in the narrow strip \( M^{\text{bnd}} \) of the manifold \( M \) near the boundary \( \partial M \) of the width \( \varepsilon_1 \) that are at the same time in a narrow strip of the width \( \varepsilon_2 \) near \( \Sigma_0 \)

\[
M_0^{\text{bnd}} = \{ x \in M \mid \text{dist}(x, \partial M) < \varepsilon_1, \text{dist}(x, \Sigma_0) < \varepsilon_2 \}. \tag{37}
\]

Further, \( M_1^{\text{bnd}} \) is the part of the thin strip \( M^{\text{bnd}} \) of the manifold \( M \) (of the width \( \varepsilon_1 \)) near the boundary \( \partial M \) that is near \( \Sigma_1 \) but on the finite distance from \( \Sigma_0 \), i.e.

\[
M_1^{\text{bnd}} = \{ x \in M \mid \text{dist}(x, \Sigma_1) < \varepsilon_1, \text{dist}(x, \Sigma_0) > \varepsilon_2 \}. \tag{38}
\]

Similarly,

\[
M_2^{\text{bnd}} = \{ x \in M \mid \text{dist}(x, \Sigma_2) < \varepsilon_1, \text{dist}(x, \Sigma_0) > \varepsilon_2 \}. \tag{39}
\]

Finally, \( M^{\text{int}} \) is the interior of the manifold \( M \) without a thin strip at the boundary \( \partial M \), i.e.

\[
M^{\text{int}} = M \setminus ( M_1^{\text{bnd}} \cup M_2^{\text{bnd}} \cup M_0^{\text{bnd}} ) = \{ x \in M \mid \text{dist}(x, \partial M) > \varepsilon_1 \}. \tag{40}
\]

We will construct the parametrix on \( M \) by using different approximations in different domains. Strictly speaking, to glue them together in a smooth way one should use ‘smooth characteristic functions’ of different domains (partition of unity) and carry out all necessary estimates. What one has to control is the order of the remainder terms in the limit \( t \to 0 \) and their dependence on \( \varepsilon_1 \) and \( \varepsilon_2 \). Since our task here is not to prove the form of the asymptotic expansion (32), which is known, but rather to compute explicitly the coefficients of the asymptotic expansion, we will not worry about such subtle details. We will compute the asymptotic expansion as \( t \to 0 \) in each domain and then take the limit \( \varepsilon_1, \varepsilon_2 \to 0 \). For a rigorous treatment see [14, 15, 27] and the references therein.
We will use different local coordinates in different domains. In $M_{\text{int}}$ we do not fix the local coordinates; our treatment will be manifestly covariant.

In $M_{1}^{\text{bnd}}$ we choose the local coordinates as follows. Let $\{\hat{e}_{i}\}$, $(i = 2, \ldots , m)$, be the local frame for the tangent bundle $T\Sigma_{1}$ and $\hat{x} = (\hat{x}^{i}) = (\hat{x}^{2}, \ldots , \hat{x}^{m})$, $(i = 2, \ldots , m)$, be the local coordinates on $\Sigma_{1}$. Let $r = \text{dist}(x, \Sigma_{1})$ be the normal distance to $\Sigma_{1}$, $(r = 0$ being the defining equation of $\Sigma_{1})$, and $\hat{N} = \partial_{r}|_{\Sigma_{1}}$ be the inward pointing unit normal to $\Sigma_{1}$. Then by using the geodesic flow we get the local frame $\{N(r, \hat{x}), e_{i}(r, \hat{x})\}$ for the tangent bundle $TM$ and the local coordinates $x = (r, \hat{x})$ on $M_{1}^{\text{bnd}}$. The geometry of $\Sigma_{1}$ is described by the extrinsic curvature $K$ (second fundamental form)

$$
\hat{\nabla}_{i}e_{j} = K_{ij}N, \quad \hat{\nabla}_{i}N = -K^{j}_{i}e_{j}.
$$

(41)

The coordinate $r$ ranges from 0 to $\varepsilon_{1}$, $0 \leq r \leq \varepsilon_{1}$. The local coordinates in $M_{2}^{\text{bnd}}$ are chosen similarly.

Finally, in $M_{0}^{\text{bnd}}$ we choose the local coordinates as follows. Let $\{\hat{e}_{a}(\hat{x})\}$, $(a = 3, \ldots , m)$, be a local frame for the tangent bundle $T\Sigma_{0}$ and let $\hat{x} = (\hat{x}^{a}) = (\hat{x}^{3}, \ldots , \hat{x}^{m})$ be the local coordinates on $\Sigma_{0}$. To avoid misunderstanding we should stress here that now we use the same notation $\hat{x}$ to denote coordinates on $\Sigma_{0}$ (not on the whole $\partial M$). Let $\text{dist}_{\partial M}(x, \Sigma_{0})$ be the distance from a point $x$ on $\partial M$ to $\Sigma_{0}$ along the boundary $\partial M$. Then define $y = + \text{dist}_{\partial M}(x, \Sigma_{0}) > 0$ if $x \in \Sigma_{1}$ and $y = - \text{dist}_{\partial M}(x, \Sigma_{0}) < 0$ if $x \in \Sigma_{2}$. In other words, $y = 0$ on $\Sigma_{0}$, $(r = y = 0$ being the defining equations of $\Sigma_{0})$, $y > 0$ on $\Sigma_{1}$ and $y < 0$ on $\Sigma_{2}$. Let $\hat{n}(\hat{x}) = \partial_{y}|_{\Sigma_{0}}$ be the unit normal to $\Sigma_{0}$ pointing inside $\Sigma_{1}$. Then by using the tangential geodesic flow along the boundary (that is normal to $\Sigma_{0}$) we first get the local orthonormal frame $\{n(y, \hat{x}), e_{a}(y, \hat{x})\}$ for the tangent bundle $T\partial M$. Further, let the unit normal vector field to the boundary $\hat{N}(y, \hat{x})$ be defined as above. Then by using the normal geodesic flow to the boundary we get the local frame $\{N(r, y, \hat{x}), n(r, y, \hat{x}), e_{a}(r, y, \hat{x})\}$ for the tangent bundle $TM$ and local coordinates $(r, y, \hat{x})$ on $M_{0}^{\text{bnd}}$. The geometry of $\Sigma_{0}$ (codimension 2 manifold) is described by two extrinsic curvatures $K$ and $L$ and an additional vector $T$:

$$
\hat{\nabla}_{a}e_{b} = K_{ab}n + L_{ab}N.
$$

(42)

$$
\hat{\nabla}_{a}n = -K^{b}_{a}e_{b} + T_{a}N, \quad \hat{\nabla}_{a}N = -L^{b}_{a}e_{b} - T_{a}n.
$$

(43)

The ranges of the coordinates $r$ and $y$ are: $0 \leq r \leq \varepsilon_{1}$ and $-\varepsilon_{2} \leq y \leq \varepsilon_{2}$. Finally, we introduce the polar coordinates

$$
r = \rho \cos \theta, \quad y = \rho \sin \theta.
$$

(44)
The angle $\theta$ ranges from $-\pi/2$ to $\pi/2$ with $\theta = -\pi/2$ on $\Sigma_1$ and $\theta = \pi/2$ on $\Sigma_2$. To cover the whole $M^\text{bnd}_0$, $\rho$ should range from 0 to some $\varepsilon_3$ (depending on $\varepsilon_1$ and $\varepsilon_2$), $0 \leq \rho \leq \varepsilon_3$.

4.2 Interior Parametrix

This is the easiest case. The construction of the parametrix goes along the same lines as for manifolds without boundary (see, e.g. [19, 30, 4, 9, 43]). The basic case (when the coefficients of the operator $F$ are frozen at a point $x_0$) is, in fact, zero-dimensional, i.e. algebraic. By using the normal coordinates at $x_0$ and Fourier transform one easily obtains the leading heat kernel

$$U^\text{int}_0(t|x, x') = (4\pi t)^{-m/2} \exp \left(-\frac{|x-x'|^2}{4t}\right).$$ (45)

We try to find the fundamental solution of the heat equation near diagonal for small $t$, i.e. $x \to x'$ and $t \to 0^+$, that, instead of the boundary conditions satisfies asymptotic condition at infinity. This means that effectively one introduces a small expansion parameter $\varepsilon$ reflecting the fact that the points $x$ and $x'$ are close to each other and the parameter $t$ is small. This can be done by fixing a point $x_0 = x'$ in $M^\text{int}$, choosing the normal coordinates at this point (with $g_{\mu\nu}(x') = \delta_{\mu\nu}$), scaling

$$x \to x' + \varepsilon(x - x'), \quad y \to x' + \varepsilon(y - x'), \quad t \to \varepsilon^2 t,$$ (46)

and expanding in a power series in $\varepsilon$. We will label the scaled objects by $\varepsilon$, e.g. $U^\varepsilon$. The scaling parameter $\varepsilon$ will be considered as a small parameter in the theory and we will use it to expand everything in power (asymptotic) series in $\varepsilon$. At the very end of calculations we set $\varepsilon = 1$. The non-scaled objects, i.e. those with $\varepsilon = 1$, will not have the label $\varepsilon$. Another way of doing this is by saying that we will expand all quantities in the homogeneous functions of $(x - x')$, $(y - y')$ and $\sqrt{t}$. This construction is standard and we do not repeat it here.

One can also use instead a manifestly covariant method [19, 30, 4, 9, 43], which gives a convenient formula for the asymptotics as $t \to 0^+$

$$U^\text{int}(t) \sim \exp \left(-\frac{\sigma}{2t}\right) \Delta_1^{1/2} \sum_{k=0}^{\infty} t^{(k-m)/2} a_k,$$ (47)
where $\sigma = \sigma(x, x') = (1/2)[\text{dist}(x, x')]^2$ is one half of the square of the geodesic distance between $x'$ and $x$, $\Delta = \Delta(x, x') = g^{-1/2}(x)g^{-1/2}(x')$ is the corresponding Van Vleck-Morette determinant, $g = \det g_{\mu\nu}$, and $a_k = a_k(x, x')$ are the off-diagonal heat-kernel coefficients (note that odd order coefficients vanish identically, i.e. $a_{2k+1} = 0$). These coefficients satisfy certain differential recursion relations which can be solved in form of a covariant Taylor series near diagonal $[1]$.

The asymptotic expansion of the heat kernel on the diagonal reads

$$U_{\text{diag}}^\text{int}(t) \sim \sum_{k=0}^{\infty} t^{(k-m)/2} a_k^{\text{diag}},$$

where $a_k^{\text{diag}}(x) = a_k(x, x)$. This asymptotic expansion can be integrated over the interior of the manifold $M_{\text{int}}$. Since both the local interior coefficients $a_k$ and the volume element $d\text{vol}_g$ are regular at the boundary, these integrals have well defined limits as $\varepsilon_1 \to 0$

$$\lim_{\varepsilon_1 \to 0^+} \int_{M_{\text{int}}} \text{tr}_V a_k^{\text{diag}} = \int_M \text{tr}_V a_k^{\text{diag}}. \quad (49)$$

Thus we obtain the local interior contribution to the global heat kernel coefficients $B_k$:

$$b^{(0)}_{2k} = \text{tr}_V a_{2k}^{\text{diag}}. \quad (50)$$

As we already noted above all odd order coefficients vanish, $b^{(0)}_{2k+1} = 0$. The explicit formulas for even order coefficients $b^{(0)}_{2k}$ are known up to $b^{(0)}_8$ $[\Pi, \Theta]$. The first two coefficients have the well known form

$$b^{(0)}_0 = (4\pi)^{-m/2} \dim V, \quad (51)$$

$$b^{(0)}_2 = (4\pi)^{-m/2} \text{tr}_V \left( Q - \frac{1}{6} R \right), \quad (52)$$

where $R$ is the scalar curvature.

### 4.3 Dirichlet Parametrix

In this section we will follow closely the ideas of the paper $[\Pi]$. For an elliptic boundary-value problem the diagonal of the parametrix $U_{\text{diag}}^\text{bd}(t)$ in $M_{\text{bd}}^\text{int}$ has
exponentially small terms, i.e. of order $\sim \exp(-r^2/t)$, (recall that $r$ is the normal geodesic distance to the boundary) as $t \to 0^+$ and $r > 0$. These terms do not contribute to the asymptotic expansion of the heat-kernel diagonal outside the boundary as $t \to 0^+$. However, they behave like distributions near the boundary, and, therefore, the integrals over $M_{1}^{\text{bnd}}$, more precisely, the integrals $\lim_{\varepsilon_1 \to 0} \int_{\varepsilon_1}^{r_{1}} \int_{0}^{t} dr(...)$, do contribute to the asymptotic expansion with coefficients being the integrals over $\Sigma_1$. It is this phenomenon that leads to the boundary terms in the heat kernel coefficients. Thus, such terms determine the local boundary contributions $b_{1}^{(1)}$ to the global heat-kernel coefficients $B_{k}$. The same applies to the Neumann parametrix and $\Sigma_2$.

The Dirichlet parametrix $U_{0}^{\text{bnd},(1)}(t|x, x')$ in $M_{1}^{\text{bnd}}$ is constructed as follows. Now we want to find the fundamental solution of the heat equation near diagonal, i.e. for $x \to x'$ and for small $t \to 0$ in the region $M_{1}^{\text{bnd}}$ close to the boundary, i.e. for small $r$ and $r'$, that satisfies Dirichlet boundary conditions on $\Sigma_1$ and asymptotic condition at infinity. We fix a point on the boundary, $x_0 \in \Sigma_1$, and choose normal coordinates on $\Sigma_1$ at this point (with $g_{ij}(0, \hat{x}_0) = \delta_{ij}$).

The basic case here (when the coefficients of the operator $F$ are frozen at the point $x_0$ is one-dimensional. The zeroth-order term $U_{0}^{\text{bnd},(1)}$ is defined by the heat equation
\[
(\partial_t + F_0)U_{0}^{\text{bnd},(1)} = 0,
\] (53)
where
\[
F_0 = -\partial_r^2 - \hat{\partial}^2,
\] (54)
the initial condition
\[
U_{0}^{\text{bnd},(1)}(0|r, \hat{x}; r', \hat{x}') = \delta(r-r')\delta(\hat{x}, \hat{x}'),
\] (55)
the boundary conditions,
\[
U_{0}^{\text{bnd},(1)} \big|_{\Sigma_1} = 0,
\] (56)
and the asymptotic condition
\[
\lim_{r \to \infty} U_{0}^{\text{bnd},(1)}(t|r, \hat{x}; r', \hat{x}') = \lim_{r' \to \infty} U_{0}^{\text{bnd},(1)}(t|r, \hat{x}; r', \hat{x}') = 0.
\] (57)
Note that the restriction to the boundary (\ldots) $\big|_{\Sigma_1}$ applies only to the first argument, i.e. $r \to 0$. The operator $F_0$ is a partial differential operator.
with constant coefficients. By using the Fourier transform in the boundary coordinates \((\hat{x} - \hat{x}')\) it reduces to an ordinary differential operator of second order. Clearly, the \(\Sigma_0\) part factorizes and the solution to the remaining one-dimensional problem can be easily obtained by using the Laplace transform, for example. The leading order Dirichlet parametrix thus has the form

\[
U_0^{\text{bnd,(1)}}(t|r, \hat{x}; r', \hat{x}') = K(t|r, \hat{x}; r', \hat{x}') - K(t|r, \hat{x}; -r', \hat{x}')
\]

(58)

where

\[
K(t|r, \hat{x}; r', \hat{x}') = (4\pi t)^{-m/2} \exp \left( -\frac{||\hat{x} - \hat{x}'||^2 + (r - r')^2}{4t} \right),
\]

(59)

Note that in addition to the usual symmetry of the heat kernel, the Dirichlet parametrix possesses the following 'mirror symmetry'

\[
U_0^{\text{bnd,(1)}}(t|r, \hat{x}; r', \hat{x}') = -U_0^{\text{bnd,(1)}}(t|r, -\hat{x}; r', \hat{x}') = -U_0^{\text{bnd,(1)}}(t|r, \hat{x}; -r', \hat{x}')
\]

(60)

i.e. it is an odd function of the coordinates \(r\) and \(r'\) separately.

To construct the whole parametrix, we again scale the coordinates. But now we include the coordinates \(r\) and \(r'\) in the scaling

\[
\hat{x} \to \hat{x}_0 + \varepsilon(\hat{x} - \hat{x}_0), \quad \hat{x}' \to \hat{x}_0 + \varepsilon(\hat{x}' - \hat{x}_0)
\]

(61)

\[
r \to \varepsilon r, \quad r' \to \varepsilon r', \quad t \to \varepsilon^2 t.
\]

(62)

The corresponding differential operators are scaled by

\[
\hat{\partial} \to \frac{1}{\varepsilon} \hat{\partial}, \quad \partial_r \to \frac{1}{\varepsilon} \partial_r, \quad \partial_t \to \frac{1}{\varepsilon^2} \partial_t.
\]

(63)

Then, we expand the scaled operator \(F_\varepsilon\) in the power series in \(\varepsilon\), i.e.

\[
F \to F_\varepsilon \sim \sum_{n=0}^{\infty} \varepsilon^{n-2} F_n,
\]

(64)

where \(F_n\) are second-order differential operators with homogeneous symbols. Since the Dirichlet boundary operator does not contain any derivatives and has constant coefficients on \(\Sigma_1\) it does not scale at all.
The subsequent strategy is rather simple. We expand the scaled heat kernel in $\varepsilon$

$$U_{\varepsilon}^{\text{bnd,}(1)} \sim \sum_{n=0}^{\infty} \varepsilon^{2-m+n} U_n^{\text{bnd,}(1)},$$  \hspace{1cm} (65)$$

and substitute into the scaled version of the heat equation and the Dirichlet boundary condition on $\Sigma_1$. Then, by equating the like powers in $\varepsilon$ one gets an infinite set of recursive differential equations

$$(\partial_t + F_0) U_k^{\text{bnd,}(1)} = - \sum_{n=1}^{k} F_n U_{k-n}^{\text{bnd,}(1)}, \quad k = 1, 2, \ldots, \hspace{1cm} (66)$$

with the boundary conditions

$$U_k^{\text{bnd,}(1)}(t|0, \hat{x}; r', \hat{x}') = U_k^{\text{bnd,}(1)}(t|r, \hat{x}; 0, \hat{x}') = 0, \hspace{1cm} (67)$$

and the asymptotic conditions

$$\lim_{r \to \infty} U_k^{\text{bnd,}(1)}(t|r, \hat{x}; r', \hat{x}') = \lim_{r' \to \infty} U_k^{\text{bnd,}(1)}(t|r, \hat{x}; r', \hat{x}') = 0. \hspace{1cm} (68)$$

In other words, we decompose the parametrix into the homogeneous parts with respect to $(\hat{x} - \hat{x}_0)$, $(\hat{x}' - \hat{x}_0)$, $r$, $r'$ and $\sqrt{t}$, i.e.

$$U_k^{\text{bnd,}(1)}(t|r, \hat{x}; r', \hat{x}') = t^{(k-m)/2} U_k^{\text{bnd,}(1)}(1|t^{-1/2}r, \hat{x}'; t^{-1/2}r', \hat{x}'), \hspace{1cm} (69)$$

in particular, on the diagonal we have

$$U_k^{\text{bnd,}(1)}(t|r, \hat{x}; r, \hat{x}) = t^{(k-m)/2} U_k^{\text{bnd,}(1)}(1|t^{-1/2}r, \hat{x}; t^{-1/2}r, \hat{x}), \hspace{1cm} (70)$$

and, therefore,

$$U_{\text{diag}}^{\text{bnd,}(1)}(t) \sim \sum_{k=0}^{\infty} t^{(k-m)/2} U_k^{\text{bnd,}(1)}(1|t^{-1/2}r, \hat{x}; t^{-1/2}r, \hat{x}). \hspace{1cm} (71)$$

To compute the contribution to the asymptotic expansion of the trace of the heat kernel, we will need to compute the integral of $U_{\text{diag}}^{\text{bnd,}(1)}(t)$ over $M_1^{\text{bnd}}$. One should stress that the volume element should also be scaled

$$d \text{vol} (r, \hat{x}) \to d \text{vol} (\varepsilon r, \hat{x}) = d \text{vol} (0, \hat{x}) \cdot \sum_{k=0}^{\infty} \varepsilon^k \frac{r^k}{k!} g_k(\hat{x}) \hspace{1cm} (72)$$
where
\[ g_k(\hat{x}) = \frac{\partial^k}{\partial r^k} \left[ \frac{d \text{vol} (r, \hat{x})}{d \text{vol} (0, \hat{x})} \right]_{r=0}. \] (73)

Combining the above equations and changing the variable \( r = \sqrt{t}\xi \) we obtain
\[
\int M^{\text{bad}}_{\text{diag}} U^{\text{bnd},(1)}_k(t) = \int_{\Sigma_1} \int_0^{\varepsilon_1} dr \frac{d \text{vol} (r, \hat{x})}{d \text{vol} (0, \hat{x})} U^{\text{bnd},(1)}_k(t) \left| r, \hat{x} ; r, \hat{x} \right|
\]
\[
\sim \sum_{k=0}^{\infty} \varepsilon_{k-\mu}^{(k-\mu)/2} \int_{\Sigma_1} \int_0^{\varepsilon_1/\sqrt{t}} d\xi \xi \frac{1}{n!} g_n(\hat{x}) \int_0^{\varepsilon_1/\sqrt{t}} d\xi \xi^{n} U^{\text{bnd},(1)}_{k-n-1}(1|\xi, \hat{x} ; \xi, \hat{x}), \] (74)

We note that even if the coefficients \( U^{\text{bnd},(1)}_k \) satisfy the asymptotic regularity condition at \( r \to \infty \) off-diagonal, the diagonal values of them do not fall off at infinity. They have the following general form
\[ U^{\text{bnd},(1)}_k(1|\xi, \hat{x} ; \xi, \hat{x}) = P_k(\xi, \hat{x}) + Y^{(1)}_k(\xi, \hat{x}), \] (75)

where \( P_k(\xi, \hat{x}) \) are polynomials in \( \xi \) and \( Y^{(1)}_k(\xi, \hat{x}) \) are exponentially small, more precisely \( \sim \xi^\alpha \exp(-\xi^2) \) with some \( \alpha \), as \( \xi \to \infty \) (which corresponds to \( t \to 0 \)).

Obviously, the integrals over the polynomial part over \( M^{\text{bad}}_1 \) vanish after taking the asymptotic expansion as \( t \to 0 \) and the limit \( \varepsilon_1, \varepsilon_2 \to 0 \). The coefficients \( P_k \) constitute simply the ‘interior part’ of the parametrix and are not essential in computing the boundary contribution. The coefficients \( Y^{(1)}_k \), in contrary, behave like distributions near \( \Sigma_1 \). They give the \( \Sigma_1 \) contributions to the boundary heat kernel coefficients \( b^{(1)}_k \). In the limit \( t \to 0 \) the integral \( \int_{\varepsilon_1/\sqrt{t}} d\xi (\ldots) \) becomes \( \int_0^{\infty} d\xi (\ldots) \) plus an exponentially small remainder term. Then in the limit \( \varepsilon_1 \to 0 \) we obtain integrals over \( \Sigma_1 \) up to an exponentially small function that we are not interested in.

As the result we get the coefficients \( b^{(1),1}_k \) in the form
\[ b^{(1),1}_k = \sum_{n=0}^{k-1} \frac{1}{n!} g_n \int_0^{\infty} d\xi \xi^n \text{tr} \mathbf{V} Y^{(1)}_{k-n-1}(\xi, \hat{x}). \] (76)
These are the standard boundary heat kernel coefficients for Dirichlet boundary conditions. They are listed for example in [12, 13] up to $k = 4$. The first two have the form

$$b^{(1),1}_0 = 0,$$

$$b^{(1),1}_1 = -(4\pi)^{-(m-1)/2} \dim V \frac{1}{4},$$

$$b^{(1),1}_2 = (4\pi)^{-m/2} \dim V \frac{1}{3} K,$$  \hspace{1cm} (77)

where $K$ is the trace of the extrinsic curvature (second fundamental form) of the boundary.

### 4.4 Neumann Parametrix

The construction of the Neumann parametrix in $M^{\text{bnd}}_2$ is essentially the same except that now the boundary operator, in fact the endomorphism $\Lambda$, is not constant and should be also scaled, so that the scaled boundary conditions are [5, 3]

$$\left( \frac{1}{\varepsilon} \partial_r + \Lambda_\varepsilon \right) \varphi \bigg|_{\Sigma_2} = 0,$$  \hspace{1cm} (78)

where

$$\Lambda_\varepsilon \sim \sum_{k=0}^{\infty} \varepsilon^k \Lambda_k.$$  \hspace{1cm} (79)

The zeroth-order operator $F_0$ is given by the same formula (54) and the zero order boundary operator is just the standard Neumann one. The basic zero-order problem can again be easily solved by

$$U_0^{\text{bnd.}(2)}(t| r, \hat{x}; r', \hat{x}') = K(t| r, \hat{x}; r', \hat{x}') + K(t| r, \hat{x}; -r', \hat{x}')$$  \hspace{1cm} (80)

with the same kernel $K$ (59). Note that the Neumann parametrix has another mirror symmetry

$$U_0^{\text{bnd.}(2)}(t| r, \hat{x}; r', \hat{x}') = U_0^{\text{bnd.}(2)}(t| -r, \hat{x}; r', \hat{x}') = U_0^{\text{bnd.}(2)}(t| r, \hat{x}; -r', \hat{x}')\left|_{r'=r}\right.,$$  \hspace{1cm} (81)

i.e. it is an even function of the coordinates $r$ and $r'$ separately.
The construction of the parametrix goes along the same lines as in Dirichlet case. We have the recursive differential equations

\[(\partial_t + F_0)U_{k}^{\text{bnd},(2)} = -\sum_{n=1}^{k} F_n U_{k-n}^{\text{bnd},(2)}, \quad k = 1, 2, \ldots,\]  

(82)

with the boundary conditions

\[\partial_r U_{k}^{\text{bnd},(2)} \bigg|_{\Sigma_2} = -\sum_{n=1}^{k-1} \Lambda_n U_{k-n-1}^{\text{bnd},(2)} \bigg|_{\Sigma_2},\]  

(83)

and the asymptotic conditions

\[\lim_{r \to \infty} U_{k}^{\text{bnd},(2)}(t|r, \hat{x}; r', \hat{x}') = \lim_{r' \to \infty} U_{k}^{\text{bnd},(2)}(t|r, \hat{x}; r', \hat{x}') = 0.\]

(84)

As we already noted above the restriction to the boundary applies only to the first argument \(r\). One can repeat here everything said at the end of the previous subsection about Dirichlet parametrix. We have again homogeneity property

\[U_{k}^{\text{bnd},(2)}(t|r, \hat{x}; r', \hat{x}') = t^{(k-m)/2} U_{k}^{\text{bnd},(2)}(1|t^{-1/2}r, \hat{x}' + t^{-1/2}(\hat{x} - \hat{x}'); t^{-1/2}r', \hat{x}')\]  

(85)

and the following expansion for the diagonal

\[U_{\text{diag}}^{\text{bnd},(2)}(t) \sim \sum_{k=0}^{\infty} t^{(k-m)/2} U_{k}^{\text{bnd},(2)}(1|t^{-1/2}r, \hat{x}; t^{-1/2}r, \hat{x}).\]  

(86)

By separating the polynomial and exponentially small parts,

\[U_{k}^{\text{bnd},(2)}(1|\xi, \hat{x}; \hat{x}) = P_k(\xi, \hat{x}) + Y_k^{(2)}(\xi, \hat{x}),\]

(87)

and repeating the arguments at the end of the previous subsection we obtain the \(\Sigma_2\) contributions to the boundary heat kernel coefficients \(b_k^{(1,2)}\)

\[b_k^{(1,2)} = \sum_{n=0}^{k-1} \frac{1}{n! \gamma_n} \int_0^{\infty} d\xi \xi^n \text{tr} \gamma Y_{n-1}^{(2)}(\xi, \hat{x}).\]

(88)
These are the standard boundary heat kernel coefficients for Neumann boundary conditions. They are listed for example in \cite{12, 13} up to $k = 4$. The first two have the form

$$b_0^{(1),2} = 0,$$

$$b_1^{(1),2} = (4\pi)^{-(m-1)/2} \dim V \frac{1}{4},$$

$$b_2^{(1),2} = (4\pi)^{-m/2} \dim V \frac{1}{3} K.$$  \hfill (89)

\section{Mixed Parametrix}

This is the most complicated (and the most interesting) case, since here the basic problem with frozen coefficients on $\Sigma_0$ is \textit{two-dimensional}. More precisely, in $M_0^{\text{bnd}}$ the basic problem is on the half-plane. Since the origin is a singular point, we will work in polar coordinates introduced above.

\subsection{Basic Problem (Zeroth Order)}

First of all, we need to solve the basic problem for operators with frozen coefficients at a point $\hat{x}_0$ on $\Sigma_0$. We choose normal coordinates on $\Sigma_0$ at this point (with $g_{ab}(0, \theta, \hat{x}_0) = \delta_{ab}$) and the polar coordinates $(\rho, \theta)$ in the normal bundle described above. Then the zero order operator $F_0$ has the form

$$F_0 = -\partial^2_\rho - \frac{1}{\rho^2} \partial_\rho - \frac{1}{\rho^2} \partial^2_\theta - \hat{\partial}^2$$  \hfill (90)

where $\hat{\partial}^2 = \hat{g}^{ab} \hat{\partial}_a \hat{\partial}_b$. The zero order inward pointing normal $N$ to the boundary in polar coordinates has the form

$$N_0\bigg|_{\Sigma_1} = \partial_r \bigg|_{y>0} = -\frac{1}{\rho} \partial_\theta \bigg|_{\rho>0, \theta=\frac{\pi}{2}},$$  \hfill (91)

$$N_0\bigg|_{\Sigma_2} = \partial_r \bigg|_{y<0} = \frac{1}{\rho} \partial_\theta \bigg|_{\rho>0, \theta=-\frac{\pi}{2}},$$  \hfill (92)

$$N_0\bigg|_{\Sigma_0} = \partial_\rho \bigg|_{y=0} = \partial_\rho \bigg|_{\rho=0, \theta=0}.$$  \hfill (93)

Now the boundary operator is discontinuous, and there is a \textit{singularity} at the origin $\rho = 0$. 
Again the part due to $\Sigma_0$ factorizes
\[
U^{\text{bnd},(0)}_0(t|\rho,\theta;\hat{x};\rho',\theta',\hat{x}')
= (4\pi t)^{-(m-2)/2} \exp\left(-\frac{|\hat{x} - \hat{x}'|^2}{4t}\right) \Psi(t|\rho,\theta;\rho',\theta') ,
\]
where $\Psi(t|\rho,\theta;\rho',\theta')$ is a two-dimensional heat kernel. It is determined by
the heat equation
\[
\left( \partial_t - \partial^2_\rho - \frac{1}{\rho} \partial_\rho - \frac{1}{\rho^2} \partial^2_\theta \right) \Psi(t|\rho,\theta;\rho',\theta') = 0 ,
\]
the initial condition
\[
\Psi(0^+|\rho,\theta;\rho',\theta') = \frac{1}{\sqrt{\rho \rho'}} \delta(\rho - \rho') \delta(\theta - \theta') ,
\]
the boundary conditions
\[
\Psi(t|\rho,\theta;\rho',\theta') \bigg|_{\theta = \pi} = 0 ,
\]
\[
\partial_\theta \Psi(t|\rho,\theta;\rho',\theta') \bigg|_{\theta = -\pi} = 0 ,
\]
the symmetry condition
\[
\Psi(t|\rho,\theta;\rho',\theta') = \Psi(t|\rho',\theta';\rho,\theta) ,
\]
as well as some boundary conditions at $\rho \to 0^+$ and $\rho \to \infty$.

We require certain regularity conditions at infinity,
\[
\int_0^\infty d\rho \sqrt{\rho \rho'} |\Psi(t|\rho,\theta;\rho',\theta')| < \infty ,
\]
in particular,
\[
\lim_{\rho \to \infty} \sqrt{\rho \rho'} \Psi(t|\rho,\theta;\rho',\theta') = \lim_{\rho \to \infty} \partial_\rho \left[ \sqrt{\rho \rho'} \Psi(t|\rho,\theta;\rho',\theta') \right] = 0 .
\]

As far as the boundary condition on $\Sigma_0$, i.e. at $\rho = 0$, is concerned, we will see that it cannot be a generic condition, rather, like for the usual
Frobenius theory of differential equations near singular points, one has a couple of possibilities for the type of singularity that need to be specified.

Since we are looking for the solution of the heat equation whose diagonal is integrable near boundary, we require

\[ \int_0^{\varepsilon_3} d\rho \rho |\Psi(t|\rho, \theta; \rho, \theta)| < \infty. \] (102)

This effectively imposes a restriction on the type of the singularity at \( \rho \to 0 \), i.e. the singularity of the heat kernel at \( \rho \to 0 \) must be weaker than \( (\rho \rho')^{-1} \). More precisely, we assume that

\[ \sqrt{\rho \rho'} |\Psi(t|\rho, \theta; \rho', \theta')| < \infty. \] (103)

We will see that this is still not enough to fix a unique solution and another boundary condition at \( \rho \to 0 \) is needed. Since the point \( \rho = 0 \) is singular, this boundary condition cannot be imposed arbitrarily. Also it does not follow from the boundary conditions on \( \Sigma_1 \) and \( \Sigma_2 \). We impose it in one of the following forms

\[ \left[ \sqrt{\rho \rho'} \Psi(t|\rho, \theta; \rho', \theta') \right] \bigg|_{\rho=0^+} = 0, \] (104)

or

\[ (\partial_\rho - s) \left[ \sqrt{\rho \rho'} \Psi(t|\rho, \theta; \rho', \theta') \right] \bigg|_{\rho=0^+} = 0, \] (105)

where \( s \) is a real parameter. We will see that the heat kernel asymptotics do depend on this boundary condition as well. We call the boundary condition (104) “regular” boundary condition. It corresponds formally to the limit \( s \to \infty \).

To construct the heat kernel we study first the operator

\[ L = -\partial_\theta^2 \] (106)

on the interval \([-\pi/2, \pi/2]\) with the boundary conditions

\[ \varphi(\theta) \big|_{\theta=\pi/2} = 0, \quad \partial_\theta \varphi(\theta) \big|_{\theta=-\pi/2} = 0. \] (107)

It is not difficult to find the spectral resolution of this operator. Its orthonormal eigenfunctions and eigenvalues are

\[ \varphi_n(\theta) = \sqrt{\frac{2}{\pi}} \cos \left[ \left( n + \frac{1}{2} \right) \left( \theta + \frac{\pi}{2} \right) \right], \] (108)
\[\lambda_n = \left(n + \frac{1}{2}\right)^2, \quad (109)\]

where \(n = 0, 1, 2, \ldots\)

By separating the variables

\[\Psi(t|\rho, \theta; \rho', \theta') = \sum_{n=0}^{\infty} \varphi_n(\theta)\varphi_n(\theta')u_n(t|\rho; \rho') \quad (110)\]

we obtain the equation

\[\left[\partial_t - \partial_\rho^2 - \frac{1}{\rho}\partial_\rho + \frac{1}{\rho^2} \left(n + \frac{1}{2}\right)^2\right]u_n(t|\rho; \rho') = 0, \quad (111)\]

with the initial condition

\[u_n(0^+|\rho; \rho') = \frac{1}{\sqrt{\rho\rho'}}\delta(\rho - \rho'), \quad (112)\]

the symmetry condition

\[u_n(t|\rho; \rho') = u_n(t|\rho'; \rho) \quad (113)\]

and the asymptotic conditions at infinity

\[\int_0^{\infty} d\rho \sqrt{\rho\rho'} \ |u_n(t|\rho, \theta; \rho', \theta')| < \infty, \quad (114)\]

\[\lim_{\rho \to \infty} \sqrt{\rho\rho'} \ u_n(t|\rho; \rho') = \lim_{\rho \to \infty} \partial_\rho \left[\sqrt{\rho\rho'} \ u_n(t|\rho; \rho')\right] = 0. \quad (115)\]

The boundary conditions at \(\rho = 0\) are

\[\sqrt{\rho\rho'} |u_n(t|\rho, \rho')| < \infty, \quad (116)\]

and, more precisely, one of the following

\[\left[\sqrt{\rho\rho'} \ u_n(t|\rho, \theta; \rho', \theta')\right]_{\rho=0^+} = 0, \quad (117)\]

or

\[(\partial_\rho - s) \left[\sqrt{\rho\rho'} \ u_n(t|\rho, \theta; \rho', \theta')\right]_{\rho=0^+} = 0. \quad (118)\]
Let us consider the operator

\[ D_n = -\partial^2_\rho - \frac{1}{\rho} \partial_\rho + \frac{1}{\rho^2} \left( n + \frac{1}{2} \right)^2. \]  

(119)

It has the “eigenfunctions” \( J_\nu(\mu \rho) \):

\[ D_n J_\nu(\mu \rho) = \mu^2 J_\nu(\mu \rho), \]

(120)

where \( \mu \) is a positive real parameter, \( J_\nu(z) \) are Bessel functions of the first kind of order \( \nu \), and \( \nu \) can take one of two values, either \( \nu = (n + \frac{1}{2}) \) or \( \nu = -(n + \frac{1}{2}) \). However, the behavior at \( \rho \to 0 \) of the Bessel function \( J_{-(n+\frac{1}{2})}(\mu \rho) \) for \( n \geq 1 \) is too singular, \( \sim \rho^{-(n+\frac{1}{2})} \), which violates the integrability condition (116). This means that for any \( n \geq 1 \) we have to choose \( \nu = (n + \frac{1}{2}) \). Note that these are not “true” eigenfunctions, since they are non-normalizable. Rather they satisfy the following “orthogonality” condition

\[ \int_0^\infty d\mu \mu J_{n+\frac{1}{2}}(\mu \rho)J_{n+\frac{1}{2}}(\mu \rho') = \frac{1}{\sqrt{\rho \rho'}} \delta(\rho - \rho'). \]

(121)

In the case \( n = 0 \) both choices are possible, i.e. \( \nu = +1/2 \) or \( \nu = -1/2 \), which makes the analysis of the problem more complicated. Therefore, we will treat the cases \( n \geq 1 \) and \( n = 0 \) separately.

**Case I.** We consider first the case \( n \geq 1 \). We will solve this problem by employing the Hankel transform which is well defined in the class of functions satisfying the conditions imposed above. We define

\[ v_n(t|\mu, \rho') = \int_0^\infty d\rho \rho J_{n+\frac{1}{2}}(\mu \rho)u_n(t|\rho, \rho'), \]

(122)

then

\[ u_n(t|\rho, \rho') = \int_0^\infty d\mu \mu J_{n+\frac{1}{2}}(\mu \rho)v_n(t|\mu, \rho'), \]

(123)

Next, by integrating by parts and using the eq. (120), we compute the Hankel transform

\[ \int_0^\infty d\rho \rho J_{n+\frac{1}{2}}(\mu \rho)D_n u_n(t|\rho, \rho') = \mu^2 \int_0^\infty d\rho \rho J_{n+\frac{1}{2}}(\mu \rho)u_n(t|\rho, \rho') \]
Finally, by taking into account the boundary conditions \((113)\) and \((116)\), and the asymptotic form of the Bessel functions, we obtain
\[
\int_0^\infty d\rho \rho J_{n+\frac{1}{2}}(\mu \rho) D_n u_n(t|\rho, \rho') = \mu^2 v_n(t|\mu, \rho').
\]
(125)

Thus, the Hankel transform of the heat equation \((111)\) is
\[
(\partial_t + \mu^2) v_n(t|\mu, \rho') = 0.
\]
(126)

From \((112)\) we also obtain the initial condition
\[
v_n(0^+|\mu, \rho') = J_{n+\frac{1}{2}}(\mu \rho').
\]
(127)

It immediately follows that
\[
v_n(t|\mu, \rho') = e^{-t\mu^2} J_{n+\frac{1}{2}}(\mu \rho'),
\]
(128)

and, therefore,
\[
u_n(t|\mu, \rho') = \frac{1}{2t} e^{-t\mu^2} J_{n+\frac{1}{2}}(\mu \rho').
\]
(129)

This integral can be computed by using the properties of the Bessel functions. We obtain finally
\[
u_n(t|\mu, \rho') = \frac{1}{2t} \exp \left( -\frac{\rho^2 + \rho'^2}{4t} \right) I_{n+1/2} \left( \frac{\rho \rho'}{2t} \right),
\]
(130)

where \(I_{n+1/2}(z)\) is the modified Bessel function of first kind. Note that this solution satisfies both boundary conditions \((117)\) and \((118)\).

CASE II. Now let us consider the case \(n = 0\). As we have seen the condition of integrability \((116)\) does not fix the solution uniquely, since there are two linearly independent solutions that satisfy that condition, which corresponds to the choices \(\nu = -1/2\) and \(\nu = +1/2\). The Hankel transform in this
case reduces to the standard cosine and sine Fourier transforms. However, we will not use them, but will solve the heat equation directly.

Let us single out the allowed singular factor

$$u_0(t|\rho, \rho') = \frac{1}{\sqrt{\rho \rho'}} w(t|\rho, \rho'). \quad (131)$$

Then, the heat equation (111), the initial condition (112), and the boundary conditions (117) and (118) take the form

$$\left( \partial_t - \partial^2_{\rho} \right) w(t|\rho, \rho') = 0, \quad (132)$$

$$w(0^+|\rho, \rho') = \delta(\rho - \rho') \quad (133)$$

$$w(t|\rho, \rho') \big|_{\rho=0} = 0, \quad (134)$$

or

$$\left( \partial_{\rho} - s \right) w(t|\rho, \rho') \big|_{\rho=0} = 0. \quad (135)$$

There is also the usual regularity condition at infinity $\rho \to \infty$.

As we see, $w$ is just the standard one-dimensional heat kernel on the half-axis. By using the Laplace transform we easily obtain the solution of this problem

$$w(t|\rho, \rho') = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\lambda e^{-t\lambda} \frac{1}{2\sqrt{-\lambda}} \left\{ \exp \left[ -\sqrt{-\lambda} |\rho - \rho'| \right] + \sqrt{-\lambda - s} \exp \left[ -\sqrt{-\lambda}(\rho + \rho') \right] \right\}, \quad (136)$$

where $c$ is a sufficiently large negative real constant, i.e. $\sqrt{-c} > -s$, and $\sqrt{-\lambda}$ is defined in the complex plane of $\lambda$ with a cut along the real positive half-axis, so that $\text{Re} \sqrt{-\lambda} > 0$. Notice that the boundary conditions (134) correspond to the limit $s \to +\infty$. The limit $s \to -\infty$ is not well defined since the constant $c$ depends on $s$ and would have to go to $-\infty$ as well.

Next, let us change the variable $\lambda$ according to

$$\lambda = \mu^2, \quad \mu = i\sqrt{-\lambda}, \quad (137)$$

where $\text{Im} \mu > 0$. In the upper half-plane, $\text{Im} \mu > 0$, this change of variables is single-valued and well defined. Under this change the complex $\lambda$-plane is

...
mapped onto the upper half $\mu$-plane, and the cut in the complex $\lambda$-plane along the positive real axis from 0 to $\infty$ is mapped onto the whole real axis in the $\mu$-plane.

The contour of integration in the complex $\mu$-plane is a hyperbola going from $(e^{i3\pi/4})\infty$ through the point $\sqrt{-c}$ to $(e^{i\pi/4})\infty$. It can be deformed to a contour $C$ that is above all poles of the integrand. It comes from $-\infty$ along the real axis, encircles possible poles on the imaginary axis in the clockwise direction, and goes to $+\infty$ along the real axis.

After such a transformation we obtain

$$w(t|\rho,\rho') = \int_C \frac{d\mu}{2\pi} \left\{ \exp \left[ -t\mu^2 + i\mu|\rho - \rho'| \right] + \frac{\mu - is}{\mu + is} \exp \left[ -t\mu^2 + i\mu(\rho + \rho') \right] \right\}. \quad (138)$$

This function is an analytic function of $s$ since the contour $C$ is above the pole at $-is$. Therefore, we can compute it, for example, for $s > 0$, and then make an analytical continuation on the whole complex $s$-plane. So, let $s > 0$. Then the pole $-is$ is in the lower half-plane. Therefore, the contour $C$ can be deformed to just the real axis, i.e. $-\infty < \mu < \infty$. Next, we use the following trick

$$\frac{\mu - is}{\mu + is} = 1 - 2is \frac{1}{\mu + is} = 1 - 2s \int_0^\infty dp e^{ip(\mu + is)}. \quad (139)$$

This integral converges since $s > 0$. Substituting this equation in (138) and evaluating the Gaussian integral over $\mu$, we obtain

$$w(t|\rho,\rho') = (4\pi t)^{-1/2} \left\{ \exp \left[ -\frac{(\rho - \rho')^2}{4t} \right] + \exp \left[ -\frac{(\rho + \rho')^2}{4t} \right] 
- 2s \int_0^\infty dp \exp \left[ -\frac{(\rho + \rho' + p)^2}{4t} - ps \right] \right\}, \quad (140)$$

which can be expressed in terms of the complimentary error function

$$w(t|\rho,\rho') = (4\pi t)^{-1/2} \left\{ \exp \left[ -\frac{(\rho - \rho')^2}{4t} \right] + \exp \left[ -\frac{(\rho + \rho')^2}{4t} \right] 
- 2\sqrt{\pi} s \sqrt{t} \exp \left[ ts^2 + (\rho + \rho')s \right] \text{erfc} \left( \frac{\rho + \rho'}{2\sqrt{t}} + s\sqrt{t} \right) \right\}. \quad (141)$$
Here \( \text{erfc}(z) \) is defined by
\[
\text{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_{z}^{\infty} du e^{-u^2}.
\]

\( (142) \)

The case \( s < 0 \) can be analyzed either directly or by the analytical continuation. The direct computation is different since now the pole \(-is\) is in the upper half-plane and one has to take into account the residue at this pole. However, the integral along the real axis is also different, so that the sum is the same. In other words, the result for \( s < 0 \) has the same analytical form (141).

Finally, we obtain the heat kernel component \( u_0 \):
\[
u(t|\rho,\rho') = (4\pi t)^{-1/2} \frac{1}{\sqrt{\rho \rho'}} \left\{ \exp \left[ -\frac{(\rho - \rho')^2}{4t} \right] + \exp \left[ -\frac{(\rho + \rho')^2}{4t} \right] \right\} - 2\sqrt{\pi} s \sqrt{t} \exp [ts^2 + (\rho + \rho')s] \text{erfc} \left( \frac{\rho + \rho'}{2\sqrt{t}} + s\sqrt{t} \right) \}.
\]

\( (143) \)

In the particular case \( s = 0 \) we get
\[
u_0(t|\rho,\rho') = (4\pi t)^{-1/2} \frac{1}{\sqrt{\rho \rho'}} \left\{ \exp \left[ -\frac{(\rho - \rho')^2}{4t} \right] + \exp \left[ -\frac{(\rho + \rho')^2}{4t} \right] \right\}.
\]

\( (144) \)

The case \( s \to +\infty \) corresponds to the regular boundary conditions (117). In this case the solution reads
\[
u_0(t|\rho,\rho') = (4\pi t)^{-1/2} \frac{1}{\sqrt{\rho \rho'}} \left\{ \exp \left[ -\frac{(\rho - \rho')^2}{4t} \right] - \exp \left[ -\frac{(\rho + \rho')^2}{4t} \right] \right\} - \frac{1}{2t} \exp \left( -\frac{\rho^2 + \rho'^2}{4t} \right) I_{1/2} \left( \frac{\rho \rho'}{2t} \right),
\]

\( (145) \)

and coincides with the solution (130) for \( n = 0 \) obtained by the Hankel transform.

Combining our results and using the explicit form of the eigenfunctions \( \varphi_n \), we obtain the heat kernel
\[
\Psi(t|\rho,\theta;\rho',\theta') = (4\pi t)^{-1} \Phi(t|\rho,\rho')
\]
\[
\times \left\{ \cos \left( \frac{\theta - \theta'}{2} \right) + \cos \left( \frac{\theta + \theta' + \pi}{2} \right) \right\} \\
+ (4\pi t)^{-1} \exp \left( -\frac{\rho^2 + \rho'^2}{4t} \right) \\
\times \left\{ \Omega \left( \frac{\rho \rho'}{2t}, \theta - \theta' \right) + \Omega \left( \frac{\rho \rho'}{2t}, \theta + \theta' + \pi \right) \right\} ,
\]

(146)

where

\[
\Phi(t|\rho, \theta; \rho', \theta') = 4 \sqrt{\pi} \left( \frac{t}{\rho \rho'} \right)^{1/2} \left\{ \exp \left[ -\frac{(\rho + \rho')^2}{4t} \right] \\
- \sqrt{\pi} s \sqrt{t} \exp \left[ ts^2 + (\rho + \rho')s \right] \text{erfc} \left( \frac{\rho + \rho'}{2\sqrt{t}} + s\sqrt{t} \right) \right\} ,
\]

(147)

and

\[
\Omega(z, \gamma) = 2 \sum_{n=0}^{\infty} I_{n+1/2}(z) \cos \left( n + \frac{1}{2} \right) \gamma .
\]

(148)

Notice that for the “regular” boundary conditions (104), which correspond to the limit \( s \to +\infty \), the function \( \Phi(t|\rho, \rho') \) vanishes.

This series can be evaluated by using the following integral representation of the Bessel function

\[
I_{n+1/2}(z) = \frac{1}{\sqrt{\pi} n!} \left( \frac{z}{2} \right)^{n+1/2} \int_{-1}^{1} dp \, e^{-p^2} (1 - p^2)^n .
\]

(149)

Substituting this integral in the series and summing over \( n \) we obtain

\[
\Omega(z, \gamma) = \sqrt{\frac{z}{2\pi}} \int_{-1}^{1} dp \, e^{-p^2} \left\{ \exp \left[ \frac{1}{2} (1 - p^2) z e^{i\gamma} + \frac{1}{2} i\gamma \right] \\
+ \exp \left[ \frac{1}{2} (1 - p^2) z e^{-i\gamma} - \frac{1}{2} i\gamma \right] \right\} .
\]

(150)

The remaining integral can be expressed in terms of the error function, so that finally we get

\[
\Omega(z, \gamma) = e^{z \cos \gamma} \text{erf} \left[ \sqrt{2z} \cos \left( \frac{\gamma}{2} \right) \right]
\]

(151)
where the error function is defined by

\[ \text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z dp e^{-p^2}. \]  

(152)

By adding the \( \Sigma_0 \) factor we obtain the final answer for the parametrix

\[ U_{0}^{\text{bnd},(0)}(t|\rho, \theta; \rho', \theta') = L(t|\rho, \theta, \hat{x}; \rho', \theta', \hat{x}') + L(t|\rho, \theta, \hat{x}; \rho', -\theta' - \pi, \hat{x}') \]  

(153)

where

\[
\begin{align*}
L(t|\rho, \theta, \hat{x}; \rho', \theta', \hat{x}') &= (4\pi t)^{-m/2} \exp \left( -\frac{|\hat{x} - \hat{x}'|^2}{4t} \right) \Phi(t|\rho, \rho') \cos \left( \frac{\theta - \theta'}{2} \right) \\
&\quad + (4\pi t)^{-m/2} \exp \left\{ -\frac{1}{4t} \left[ |\hat{x} - \hat{x}'|^2 + \rho^2 + \rho'^2 - 2\rho \rho' \cos(\theta - \theta') \right] \right\} \\
&\quad \times \text{erf} \left( \sqrt{\frac{\rho \rho'}{t}} \cos \left( \frac{\theta - \theta'}{2} \right) \right). 
\end{align*}
\]

(154)

An important corollary from this formula are the symmetries of the heat kernel. First of all, we have the usual ‘self-adjointness’ symmetry

\[ \theta \rightarrow \theta', \quad \rho \rightarrow \rho'. \]  

(155)

Second, we have the ‘periodicity’ symmetries

\[ \theta \rightarrow \theta + 4\pi n, \quad \theta' \rightarrow \theta' + 4\pi m, \quad n, m \in \mathbb{Z}. \]  

(156)

Finally, there is additional ‘mirror’ symmetry

\[
\begin{align*}
\theta &\rightarrow \theta, \quad \theta' \rightarrow -\theta' - \pi \\
\theta &\rightarrow -\theta - \pi, \quad \theta' \rightarrow \theta' 
\end{align*}
\]

(157, 158)

Note the essential difference of the symmetries of the mixed parametrix versus those of the Dirichlet and Neumann parametrices. The mixed parametrix is a periodic function of the angles (expected), but not with the period \( 2\pi \) but with the period \( 4\pi \) (not expected). That is why there are two different mirror images, \((\rho, -\theta - \pi, \hat{x})\) and \((\rho, -\theta + \pi, \hat{x})\), of a point with the coordinates
\((\rho, \theta, \bar{x})\). In other words the double reflection of a point does not bring it back—*the double image is not identical with the original point*. Denoting by \(T\) the transformation \(\theta \to -\theta - \pi\) we have

\[
T^4 = \text{Id}, \quad \text{but} \quad T^2 \neq \text{Id}.
\] (159)

The operator \(T\) has *four* eigenvalues \(1, -1, i\) and \(-i\). Whereas the first two, 1 and \(-1\), are the standard ones, the latter two, \(i\) and \(-i\), correspond to some *new* images. This might have some interesting applications.

The diagonal of the mixed parametrix is easily found to be

\[
U^{\text{bnd},(0)}_{\text{diag},0}(t) = (4\pi t)^{-m/2} \left\{ 1 - \text{erfc} \left( \frac{\rho}{\sqrt{t}} \right) 
- \exp \left( -\frac{\rho^2 \cos^2 \theta}{t} \right) \text{erf} \left( \frac{\rho \sin \theta}{\sqrt{t}} \right) 
+ (1 - \sin \theta) \frac{4}{\sqrt{\pi}} \rho \left[ \exp \left( -\frac{\rho^2}{t} \right) 
- \sqrt{\pi} s \sqrt{t} \exp (t s^2 + 2 \rho s) \text{erfc} \left( \frac{\rho}{\sqrt{t}} + s \sqrt{t} \right) \right] \right\}. \] (160)

Now we compute the integral of the diagonal of the parametrix over \(M_0^{\text{bnd}}\)

\[
\int_{M_0^{\text{bnd}}} \text{tr}_V U^{\text{bnd},(0)}_{\text{diag},0}(t) = \int_0^{\varepsilon_3} d\rho \int_0^{\pi/2} d\theta \text{tr}_V U^{\text{bnd},(0)}_{\text{diag},0}(t) \] (161)

for some finite \(\varepsilon_3 > \sqrt{\varepsilon_1^2 + \varepsilon_2^2} > 0\).

First of all, obviously the integrals over \(\theta\) of the odd functions in \(\theta\) vanish identically. So, we only need to consider the even part. Second, since in the limit \(\varepsilon_3 \to 0\) the volume of \(M_0^{\text{bnd}}\) vanishes, the regular part of the heat kernel diagonal does not contribute to the trace either. It is only the singular part of the heat kernel diagonal, which behaves like a distribution near \(\Sigma_0\), that contributes to the integral in the limit \(\varepsilon_3 \to 0\).

The integral over \(\rho\) can be computed exactly. It reads

\[
\int_{M_0^{\text{bnd}}} \text{tr}_V U^{\text{bnd},(0)}_{\text{diag},0}(t) = \int_{\Sigma_0} (4\pi t)^{-m/2} \dim V \left( \frac{\pi \varepsilon_3^2}{2} \right) 
+ t \left[ -\frac{\pi}{4} + 2\pi \Theta \left( \sqrt{t} s \right) \right] + X(t) \right\}, \] (162)
where
\[ \Theta(z) = e^{z^2} \text{erfc}(z), \quad (163) \]
and
\[ X(t) = 2\sqrt{\pi}t \varepsilon_3 \exp \left( -\frac{\varepsilon_3^2}{t} \right) + \left( \frac{\pi t}{4} - \frac{\pi \varepsilon_3^2}{2} \right) \text{erfc} \left( \frac{\varepsilon_3}{\sqrt{t}} \right) - 2\pi t \exp (ts^2 + 2s\varepsilon_3) \text{erfc} \left( \frac{\varepsilon_3}{\sqrt{t}} + \sqrt{t}s \right). \quad (164) \]

Notice that \( \pi \varepsilon_3^2/2 \) is nothing but the area of the semi-circle of radius \( \varepsilon_3 \), so that \( \text{vol}(\Sigma_0)\pi \varepsilon_3^2/2 = \text{vol}(M^\text{bnd}_0) \). In the limit \( \varepsilon_3 \to 0 \) this term does not contribute to the asymptotics.

By using the asymptotic behavior of the error function as \( z \to \infty \)
\[ \text{erfc}(z) \sim \frac{1}{\sqrt{\pi z}} e^{-z^2}. \quad (165) \]

we find that the function \( X(t) \) is exponentially small, i.e. it is suppressed by the factor \( \sim \exp(-\varepsilon_3^2/t) \), as \( t \to 0 \), and, therefore, does not contribute to the asymptotic expansion of the heat kernel in powers of \( t \) either.

The behavior of the function \( \Theta(\sqrt{t}s) \) depends on the parameter \( s \). For a finite \( s \) in the limit \( t \to 0 \) we have
\[ \Theta \left( \sqrt{t}s \right) = 1 + O(t^{1/2}). \quad (166) \]

It immediately follows that for a finite \( s \), i.e. for the boundary conditions (103) the singular heat kernel coefficient \( b_2^{(2)} \) is equal to
\[ b_2^{(2)} = (4\pi)^{-(m-2)/2} \dim V \frac{7}{16}. \quad (167) \]

Notice that it does not depend on \( s \) explicitly.

Finally we analyze the regular boundary conditions (104), which corresponds formally to the limit \( s \to +\infty \). By using (165) we see that for a finite \( t \) the function \( \Theta(\sqrt{t}s) \) vanishes in the limit \( s \to \infty \):
\[ \Theta \left( \sqrt{t}s \right) \bigg|_{s \to \infty} = 0. \quad (168) \]

Therefore, in this case the coefficient \( b_2^{(2)} \) is
\[ b_2^{(2)} = -(4\pi)^{-(m-2)/2} \dim V \frac{1}{16}. \quad (169) \]

We see that the heat kernel coefficients \( b_k^{(2)} \) depend on the type of the additional boundary conditions, i.e. (104) vs. (103), at \( \Sigma_0 \).
5 Conclusions

We have studied Zaremba boundary value problem for second-order partial differential operators of Laplace type, when the manifold as well as the boundary are smooth and the differential operator has smooth coefficients but the boundary operator is discontinuous on the boundary, it jumps from the Dirichlet to Neumann type boundary operator. Since this problem is not smooth there could be additional logarithmic terms in the asymptotic expansion of the trace of the heat kernel (32). However, Selcey [40] has shown recently that such terms do not appear and there is classical asymptotic expansion in half-integer powers of $t$ only. This seems to contradict the conclusions of [21], where it has been shown that such an expansion with locally computable coefficients does not exist. The term ‘locally computable’ is confusing though. As we have seen the calculation of the coefficients of the asymptotic expansion of the trace of the heat kernel involves the knowledge of some global information, i.e. the spectrum (109) of the operator $L$ (106) with mixed boundary conditions. So, one could say that these coefficients are locally computable in the coordinates $\hat{x}$ and $\rho$ but are global in the coordinate $\theta$. Thus the standard asymptotic expansion in powers of $t$ (without logarithmic terms) still exists with coefficients (33), (34) given by integrals over $M$, $\Sigma_1$, $\Sigma_2$ and $\Sigma_0$. The interior coefficients, $b_k^{(0)}$, the co-dimension one coefficients, $b_k^{(1),1}$ and $b_k^{(1),2}$, are ‘locally computable’, but the co-dimension two coefficients, $b_k^{(2)}$, are ‘global’ in $\theta$ (or pseudo-local) and require new methods of calculation (e.g. like the approach of this paper). They are constructed from the local invariants on $\Sigma_0$. It is the numerical coefficients that are global.

Let us formulate briefly our main results. First of all, we provide the correct formulation of the Zaremba type boundary value problem. We find that the boundary conditions on the open sets $\Sigma_1$ and $\Sigma_2$ are not enough to fix the problem, and an additional boundary condition along the singular set $\Sigma_0$ is needed. This additional boundary condition can be considered formally as an ‘extension’ of Dirichlet conditions from $\Sigma_1$ to $\Sigma_0$, or an ‘extension’ of Neumann conditions from $\Sigma_2$ to $\Sigma_0$. However, strictly speaking the boundary conditions on $\Sigma_0$ does not follow from the boundary conditions on $\Sigma \setminus \Sigma_0$ and can be chosen rather arbitrarily. One needs some additional ‘physical’ criteria to fix this boundary condition. Second, we describe the geometry of the problem, which involves now some nontrivial geometrical quantities (normal
bundle and extrinsic curvatures) that characterize properly the imbedding of a co-dimension two submanifold $\Sigma_0$ in $M$. The higher order coefficients $b_k^{(2)}$ are invariants constructed from those geometric quantities. Next, we describe the construction of the parametrix of the heat equation in the interior of the manifold $M$, in a thin shell close to $\Sigma_1$ and $\Sigma_2$, and finally, in a thin strip close to $\Sigma_0$. We used the standard scaling device; the difference is just in what coordinates are involved in scaling. Finally, we have explicitly found the off-diagonal parametrix in $M_0^{\text{bnd}}$, the thin strip close to $\Sigma_0$, in the leading approximation, and used it to compute the first nontrivial ‘global’ coefficient, $b_2^{(2)}$, of the heat kernel asymptotic expansion. We considered two types of the additional boundary condition along $\Sigma_0$, one being the ‘extension’ Dirichlet boundary conditions (that we called regular boundary condition), and another being the ‘extension’ of the Neumann (or rather Robin) boundary conditions. We have shown that the result, i.e. the coefficient $b_2^{(2)}$, does depend on the type of the boundary condition, i.e. Dirichlet vs Neumann, but does not depend on the parameter $s$ of the Robin boundary condition (it will however contribute to the higher order coefficients).

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