NOTES ON HEAT KERNEL ASYMPTOTICS

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Abstract. These are informal notes on how one can prove the existence and asymptotics of the heat kernel on a compact Riemannian manifold with boundary. The method differs from many treatments in that neither pseudodifferential operators nor normal coordinates are used; rather, the heat kernel is constructed directly, using only a first (Euclidean) approximation and a Neumann (Volterra) series that removes the errors.

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1. Introduction

The theorem of Minakshisundaram-Pleijel on the asymptotics of the heat kernel states:

Theorem 1.1. *Let M be a compact Riemannian manifold without boundary. Then there is a unique heat kernel, that is, a function*

$$K \in C^\infty((0,\infty) \times M \times M)$$

satisfying

$$\begin{aligned} (\partial_t - \Delta_x) K(t,x,y) &= 0, \\ \lim_{t\to 0+} K(t,x,y) &= \delta_y(x). \end{aligned} \tag{1}$$

For each $x \in M$ there is a complete asymptotic expansion

$$K(t,x,x) \sim t^{-n/2}(a_0(x) + a_1(x)t + a_2(x)t^2 + \dots), \quad t \to 0. \tag{2}$$

The a_j are smooth functions on M, and $a_j(x)$ is determined by the metric and its derivatives at x.

Here, Δ_x is the Laplace-Beltrami-Operator acting in the variable x. In local coordinates it is given by[1]

$$\Delta = \sum_{i,j=1}^n g^{ij}(x)\partial_{x_i}\partial_{x_j} + \sum_{i=1}^n b_i(x)\partial_{x_i}. \tag{3}$$

The limit in the initial condition is to be understood in the weak sense; that is, for each $f \in C^\infty(M)$, the function[2] $u(t,x) = \int_M K(t,x,y)f(y)dy$ is continuous up to $t = 0$ and satisfies $u(0,x) = f(x)$. The a_j can be computed explicitly.

The asymptotic expansion holds uniformly in x (this is also part of the theorem), so that one can integrate it over $x \in M$, and – together with the spectral representation of K – this gives the result, central in inverse spectral theory, that

$$\sum_j e^{-t\lambda_j} \sim t^{-n/2} \sum_{i=0}^\infty \alpha_i t^i, \quad t \to 0+, \quad \alpha_i = \int_M a_i,$$

where the λ_j are the eigenvalues of the Laplacian.

The purpose of these notes is to give a proof of this theorem (and then, incrementally, of its generalizations to manifolds with boundary, manifolds with conical singularities...) which uses as little machinery as possible, and is conceptually natural from an analyst's point of view. The proofs in standard references use either Riemannian normal coordinates ([1], [2],[4])[3], or the theory of pseudodifferential operators with parameter ([6],[10]).

The central considerations in our treatment are those of homogeneity and locality: The basic homogeneity of the heat equation is that x scales like $\sqrt{t}$, at least

[1]It will not be needed for the main part of these notes, but for completeness recall what the coefficients mean: (g^{ij}) is the inverse matrix of the matrix (g_{ij}) which describes the metric tensor locally, and $b_i = \frac{1}{\sqrt{g}} \sum_{j=1}^n \partial_{x_j}(g^{ij}\sqrt{g})$, where $g = \det(g_{ij})$.

[2]Throughout these notes, all integrations will be with respect to the Riemannian measure, which will be denoted dx, although in local coordinates it is $\sqrt{g}dx$. This just simplifies matters a little, allowing us to avoid thinking about densities.

[3]I admit that I like this proof since it's very quick, and quite natural geometrically; our purpose here is to show that this geometry is actually not needed! In Section 2.5.3(2) this proof is described shortly.

in the leading terms (i.e. forgetting the terms imvolving b_i in (3)). This, along with the initial condition, leads one to expect that $K(t, x, y)$ should be expressible 'nicely' in terms of the new variable $X = (x - y)/\sqrt{t}$, in local coordinates. This expectation is supported by the well-known formula

$$E(t, x, y) = \frac{1}{(4\pi t)^{n/2}} e^{-|x-y|^2/4t} \tag{4}$$

for the heat kernel on $\mathbb{R}^n$, with the Euclidean metric.[4] Locality is the rapid decay of E as function of $(x - y)/\sqrt{t}$.

We will define spaces of functions, $\Psi_H^\alpha(M)$, $\alpha \in -\mathbb{N}_0/2$, which reflect this homogeneity and locality of E. The 'order' α encodes the leading power of t, and is normalized so that $E \in \Psi_H^{-1}(\mathbb{R}^n)$. The existence part of Theorem 1.1 will follow from the construction of a heat kernel $K \in \Psi_H^{-1}(M)$. The letter Ψ is supposed to show the close analogy of our approach to the parametrix construction for elliptic operators in the *pseudodifferential calculus*. In fact, the procedure is exactly the same, except that here in the heat equation context the details are much easier![5].

The reader is not assumed to be familiar with the pseudodifferential calculus. Neither will she learn it here. But still she will learn some of the main ideas involved in it, without having to bother with technicalities like distributions or oscillatory integrals.

The approach followed here was inspired by the treatment of R. Melrose in [13], Sections 7.1-7.3. We deviate from his treatment by proving a composition formula and using the Volterra series directly, instead of using a recursive procedure (which we also describe shortly in Section 2.5). Our purpose is to explain this method in simple terms, avoiding the somewhat arcane language used in Melrose's book.[6] However, the interested reader should definitely consult that book![7]

The boundary value problem is then treated in a similar manner. It is remarkable that, after initial basic homogeneity and locality considerations, only minor modifications are needed to treat this more general case. The treatment of the boundary value problem by this method seems to be new. (The 'b' in 'b-calculus', as treated in [13], Sections 7.4-7.5, also refers to a manifold with boundary, but to a different class of metrics (infinite cylindrical ends), which yields a different analysis.)

Generalizations: The method presented here works with any elliptic (in a suitable sense) operator replacing the Laplacian. That is, one can treat higher order operators and systems (i.e. operators acting between vector bundles) in the

[4]Actually, the heat kernel on $\mathbb{R}^n$ is only unique if one imposes certain growth conditions for $x - y \to \infty$. The homogeneity holds precisely in $\mathbb{R}^n$, and means that if $K(t, x, y)$ satisfies (1) then so does $\lambda^n K(\lambda^2 t, \lambda x, \lambda y)$ for any $\lambda > 0$ (recall that $\delta(\lambda x) = \lambda^{-n}\delta(x)$). Set $\lambda = t^{-1/2}$ and use uniqueness to see that K equals $t^{-n/2}$ times a function of $x/\sqrt{t}$, $y/\sqrt{t}$. Similarly, translation invariance shows that the latter is actually a function of $(x - y)/\sqrt{t}$, and rotation invariance that it is a radial function; putting this into (1) one obtains an ordinary differential equation for this function, which can be solved easily.

[5]In particular, this approach is more direct and simpler than the more standard approach in which first a parametrix for the resolvent is constructed as pseudodifferential operator with parameter, and then an inverse Laplace transform is applied to obtain the heat kernel.

[6]But keep in mind that we are doing this in hopes that a similar treatment is possible for 'singular manifolds', and for these it may well be advantageous to use this language!

[7]Essentially the same method of proof is used by McKean and Singer [12] (with many details missing).

same way. In particular, self-adjointness is not needed. See Section 2.5. (This is true at least for the part without boundary, and, with more modifications, also for boundary problems). See also [7], which has a quick treatment (in the case without boundary) using pseudodifferential operators (and a not so quick one with boundary).

Also, one can deal with limited smoothness, since the Volterra series only involves integrations. To determine the minimal smoothness required in the proof of existence, and to have a given number of terms in the expansion, is left as an exercise.

2. Manifolds without boundary

In this section we give a detailed analysis of the heat kernel on a compact Riemannian manifold without boundary. This will imply the theorem of Minakshisundaram-Pleijel.

2.1. **Outline of the proof.**

Our basic strategy in the proof of Theorem 1.1 follows the following standard pattern:

(1) Construct an approximate heat kernel (parametrix) K_1, in the sense that

$$\begin{aligned}(\partial_t - \Delta_x)K_1(t,x,y) &= R(t,x,y)\\ \lim_{t\to 0+} K_1 &= \delta_y(x)\end{aligned} \tag{5}$$

with R 'small' in a sense to be specified later.

(2) Correct K_1 to an exact heat kernel, by summing a convergent series (the Volterra series). This proves existence of a heat kernel, satisfying the asymptotics (2).

(3) Uniqueness can be derived from existence via duality (using self-adjointness), or proved via an energy estimate.

The obvious candidate for a first approximation is given by the Euclidean heat kernel (4). More precisely, if one wants the approximation to be good near $x = y$ (and near $t = 0$), for *each* y, then one should use the metric $g(y)$ here[8]. That is, if

$$E^{(g)}(t,x,y) = \frac{1}{(4\pi t)^{n/2}} e^{-|x-y|_g^2/4t}, \tag{6}$$

$|x|_g := \sum_{i,j=1}^n g_{ij}x_ix_j$, denotes the heat kernel for the 'constant' metric $g = (g_{ij})$, $g_{ij} \in \mathbb{R}$, on $\mathbb{R}^n$, then one may hope that

$$K_1(t,x,y) = E^{(g(y))}(t,x,y) \tag{7}$$

(in local coordinates on M, and then suitably patched together) is an approximation to the true heat kernel. Indeed, an easy calculation (see Proposition 2.7) shows that $(\partial_t - \Delta_x)K_1$ equals $t^{-n/2-1/2}$ times a smooth function of $t, (x-y)/\sqrt{t}, y$. This is 'good' since $\partial_t K_1$ and $\Delta_x K_1$ separately would have the more singular factor[9] $t^{-n/2-1}$.

The simple argument for the second step, how to 'iterate away the error terms', will be recalled in Section 2.3. This works most easily, and is standard, if R in (5) remains bounded as $t \to 0$. But we just saw that R can definitely not be expected to be bounded if K_1 is taken as in (7)! So we need

(1) either a better parametrix in the first step,

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[8]It is in this refinement in the very first step that, in the analogous construction of a parametrix for an elliptic operator, the pseudodifferential technique differs from (and improves upon) the classical method of (i) freezing coefficients at points in an ϵ-net on M, (ii) inverting the resulting constant coefficient operators in $\mathbb{R}^n$ and transferring the solutions to ϵ-neighborhoods of these points, and (iii) patching these local approximate solutions together. This method yields an error term of type 'small norm (for small ϵ) operator plus lower order operator'. In contrast, the ΨDO parametrix yields only a lower order, hence compact, error. While the classical method suffices to prove discreteness of the spectrum, for example, the ΨDO method is superior if one wants to obtain more refined quantitative information, for example the Weyl asymptotics with error term.

[9]We will see that, for this to be true, K_1 essentially (i.e. up to lower order terms) *has to be* chosen as in (7). So there is no guessing involved here, really!

(2) or a proof that the Volterra series works also with errors as are obtained from K_1 in (7).

We will do (2). This gives (1) also since we will show that finite partial sums of the Volterra series give arbitrarily good parametrices.

Therefore, the proof of (the existence and asymptotics part of) Theorem 1.1 boils down to defining

$$K = K_1 - K_1 * R + K_1 * R * R - \dots$$

(where K_1 is (7), $R = (\partial_t - \Delta_x)K_1$, and $*$ is defined in (15)) and proving the convergence of this series, and that it gives the desired asymptotics. The basics for this are developed in Section 2.2 (more than is really needed, but it seemed worth it to do things systematically), the convergence is proved in Section 2.3, and the proof is put together in Section 2.4. More remarks, for example on how to compute the a_i, follow in Section 2.5.

2.2. **The heat calculus.**

2.2.1. *The definition.* The salient features of the Euclidean heat kernel (4) and of the first approximation (7) are:

- the prefactor $t^{-n/2}$
- the exponential factor, which is a smooth function of $X = (x-y)/\sqrt{t}$ and y, exponentially decaying as $|X| \to \infty$.

It is quite clear, and we will compute it momentarily, that $(\partial_t - \Delta_x)K_1$ will have the same form, except for a different power of t in front. This motivates the following definition. We will use the following notation:

$$C^\infty([0,\infty)_{1/2})$$

consists of functions $f(t)$ which are smooth as functions[10] of $\sqrt{t}$, for $t \geq 0$. The symbol $D^\gamma_{\sqrt{t},X,y}$ means differentiations in $\sqrt{t}, X, y$, their number given by the multiindex γ.

Definition 2.1. *Let M be a manifold and $\alpha \leq 0$. The space $\Psi^\alpha_H(M)$ is the set of functions A on $(0,\infty)\times M^2$ satisfying:*

(a) *A is smooth,*

(b) *if $x \neq y$ then $D^\gamma_{t,x,y}A(t,x,y) = O(t^\infty)$ as $t \to 0$, for all γ, ('off diagonal decay')* [11]

(c) *for any $p \in M$ there is a local coordinate system $U \ni p$ and*

$$\tilde{A} \in C^\infty([0,\infty)_{1/2} \times \mathbb{R}^n \times U) \tag{8}$$

so that for $x, y \in U$ one has

$$A(t,x,y) = t^{-\frac{n+2}{2}-\alpha}\tilde{A}(t, \frac{x-y}{\sqrt{t}}, y). \tag{9}$$

Furthermore, $\tilde{A}$ is rapidly decaying in the second variable:

$$|D^\gamma_{\sqrt{t},X,y}\tilde{A}(t,X,y)| = O(|X|^{-\infty}), \quad |X| \to \infty, \tag{10}$$

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[10] that is, there is $g \in C^\infty(\mathbb{R})$ such that $f(t) = g(\sqrt{t})$ for all $t \geq 0$.

[11] We write '$O(t^\infty)$' instead of '$O(t^N)$ for all N'. This condition is a little more natural in our method than requiring exponential decay, $O(e^{-c/t})$ for some c, which would also work (with the corresponding change in (10)).

for all γ, uniformly for bounded t and y.

Note that (c) implies (b) for $x, y \in U$.

Clearly, $\Psi_H^\alpha \supset \Psi_H^{\alpha-1/2}$.

Remark: The funny normalization of the order α (leading to the unpleasant exponent of t in (9)) is motivated by the fact, proved below, that only with this normalization will the orders add under convolution (defined below) of such functions. Very negative α correspond to 'very smooth' (at $t=0$) kernels; this is chosen to parallel the usual notion of order in the pseudodifferential calculus.

It will be useful to have:

Definition 2.2. *Let $A \in \Psi_H^\alpha(M)$. Given coordinates as in Definition 2.1(c), the* leading term *of A, denoted*[12] *$\Phi_\alpha(A)$, is the function*

$$(X, y) \mapsto \tilde{A}(0, X, y),$$

with $\tilde{A}$ given in (9).

Note that $\tilde{A}$ is not defined uniquely by A: If $t > 0$ then $(x-y)/\sqrt{t}$ assumes only a bounded set of values! But whenever $X\sqrt{t}$ is sufficiently small then

$$\tilde{A}(t, X, y) = t^{(n+2)/2+\alpha} A(t, y + X\sqrt{t}, y), \tag{11}$$

so at least $\Phi_\alpha(A)$ is uniquely defined.

The definition of leading term depends on the choice of local coordinates (since $\tilde{A}$ does). We now analyze how.

2.2.2. *Coordinate invariance.*

Lemma 2.3. (a) *If condition (c) in Definition 2.1 holds in one coordinate system then it holds in any.*

(b) *The leading term $\Phi_\alpha(A)$ is defined invariantly as a function on the tangent bundle, rapidly decaying in the fiber direction:*

$$\Phi_\alpha(A) \in C^\infty_{\mathcal{S}(fibers)}(TM). \tag{12}$$

Proof. (a) Suppose $\psi(x) = \bar{x}$ is a coordinate change, and condition (c) holds in the $\bar{x}$-coordinate patch $\bar{U}$, with a function $\bar{\tilde{A}}(t, \bar{X}, \bar{y})$ satisfying (8), (10). We need to find a function $\tilde{A}$ with the same properties, and satisfying

$$\tilde{A}(t, \frac{x-y}{\sqrt{t}}, y) = \bar{\tilde{A}}(t, \frac{\psi(x) - \psi(y)}{\sqrt{t}}, \psi(y)) \tag{13}$$

for all x, y near p. This is easy: Choose a smooth, matrix-valued function h satisfying

$$\psi(x) - \psi(y) = h(x, y)(x - y)$$

and[13] $h(y, y) = d\psi_{|y}$, and a cutoff function $\chi \in C_0^\infty(\bar{U})$, equal to one near p, and then set

$$\tilde{A}(t, X, y) = \bar{\tilde{A}}(t, h(y + X\sqrt{t}, y)X, \psi(y))\chi(y + X\sqrt{t}), \tag{14}$$

which is clearly equivalent to (13), for $y, y + X\sqrt{t}$ near p.

[12] The letter Φ is supposed to reflect the German 'Führender Term'. Melrose calls this the normal operator.

[13] $h(x, y) = \int_0^1 d\psi_{|y+t(x-y)} dt$ will do

(b) From (14) and $h(y,y) = d\psi_y$ we have $\tilde{A}(0,X,y) = \tilde{\tilde{A}}(0, d\psi_y(X), \psi(y))$, which was to be shown.[14]

$\square$

Note that even if $\tilde{\tilde{A}}$ was smooth in t (rather than $\sqrt{t}$) then $\tilde{A}$ would still be only smooth in $\sqrt{t}$. So for a coordinate invariant definition we need to allow $\sqrt{t}$-dependence. Below we will see why in the final result, Theorem 1.1, only integral powers appear.

The higher order derivatives $\partial^m_{\sqrt{t}}\tilde{A}(0,X,y)$ are also determined by A, but depend on the choice of coordinates in a more complicated way. We won't need these here.

2.2.3. *Short exact sequence.* The following lemma is quite obvious, but central to any type of 'step by step improvement' argument:

Lemma 2.4. (a) *Let $A \in \Psi^\alpha_H$. Then $\Phi_\alpha(A) = 0$ iff $A \in \Psi^{\alpha-1/2}_H$.*

(b) *Given a function $F \in C^\infty_{\mathcal{S}(fibers)}(TM)$, and $\alpha \in \mathbb{R}$, there is $A \in \Psi^\alpha_H(M)$ having F as leading term.*

In other words, one has an exact sequence, for each α,

$$0 \to \Psi^{\alpha-1/2}_H(M) \to \Psi^\alpha_H(M) \xrightarrow{\Phi_\alpha} C^\infty_{\mathcal{S}(\text{fibers})}(TM) \to 0.$$

2.2.4. *Composition.* We now prove that Ψ^α_H behaves well under composition of operators. As we will see in Section 2.3, the appropriate notion of composition here is:

Definition 2.5. *The* convolution product *of two smooth functions A, B on $(0,\infty)\times M^2$ is the function, on the same space,*

$$(A * B)(t,x,y) = \int_0^t \int_M A(t-s,x,z)B(s,z,y)\,dzds, \tag{15}$$

whenever the integrals are absolutely convergent.

If one considers functions $A(t,x,y)$ as Schwartz kernels of time-dependent families of operators via $(A(t)f)(x) = \int_M A(t,x,y)f(y)\,dy$, and if one sets $A(t) = 0$ for $t < 0$ then this is just the usual convolution of functions on $\mathbb{R}$ valued in a ring (the ring of operators). Equivalently, if one associates with $A(t,x,y)$ the operator on $\mathbb{R}\times M$ whose Schwartz kernel is $(s,t,x,y) \mapsto A(t-s,x,y)H(t-s)$ (where H is the characteristic function of the positive half line) then $*$ is just composition on the level of such Schwartz kernels.

Proposition 2.6. *Let $A \in \Psi^\alpha_H(M)$, $B \in \Psi^\beta_H(M)$, with $\alpha, \beta < 0$, and assume M is compact. Then $A * B$ is defined and lies in $\Psi^{\alpha+\beta}_H(M)$. The leading terms $a = \Phi_\alpha(A)$, $b = \Phi_\beta(B)$, $a * b := \Phi_{\alpha+\beta}(A * B)$ satisfy*

$$(a * b)(X,y) = \int_0^1 \int_{\mathbb{R}^n} (1-\sigma)^{-(n+2)/2-\alpha}\sigma^{-(n+2)/2-\beta} a\Big(\frac{X-Z}{\sqrt{1-\sigma}}, y\Big) b\Big(\frac{Z}{\sqrt{\sigma}}, y\Big)\,dZd\sigma. \tag{16}$$

[14] One could have defined the leading term without reference to coordinates, as follows: Let $X \in T_yM$ be the equivalence class of a curve γ, that is $\gamma(0) = y$, $\gamma'(0) = X$. Then $\Phi_\alpha(A)(X,y) = \lim_{t\to 0} t^{(n+2)/2+\alpha}A(t,\gamma(\sqrt{t}),y)$.

Proof. First, consider x, y in a coordinate patch U, where A, B have representations as in (9) (note that we use invariance here!), and consider the part of the convolution product with z near y, that is

$$\int_0^t \int_{\mathbb{R}^n} A(t-s,x,z)B(s,z,y)\chi(z)\,dzds \tag{17}$$

where $\chi \in C_0^\infty(U)$ is equal to one near y. We replace the integration variables by $\sigma = s/t$, $Z = (z-y)/\sqrt{t}$ and introduce the new variable $X = (x-y)/\sqrt{t}$ instead of x. Then (17) becomes $t^{-(n+2)/2-\alpha-\beta}\tilde{C}(t,X,y)$ where $\tilde{C}(t,X,y)$ equals

$$\begin{aligned} &\int_0^1 \int_{\mathbb{R}^n} (1-\sigma)^{-(n+2)/2-\alpha}\sigma^{-(n+2)/2-\beta}\cdot \\ &\qquad \tilde{A}(t(1-\sigma), \frac{X-Z}{\sqrt{1-\sigma}}, y+Z\sqrt{t})\tilde{B}(t\sigma, \frac{Z}{\sqrt{\sigma}}, y)\,\chi(y+Z\sqrt{t})\,dZ\,d\sigma. \end{aligned} \tag{18}$$

Convergence and rapid decay as $|X| \to \infty$ follow for the part $\sigma \leq 1/2$ by introducing the variable $W = Z/\sqrt{\sigma}$ for Z, then the power of σ is $-1-\beta$, so the integral converges since $\beta < 0$, and rapid decay as $|X| \to \infty$ can be easily seen from $|\frac{X-W\sqrt{\sigma}}{\sqrt{1-\sigma}}| \geq ||X|-|W||$ and rapid decay of $\tilde{A}, \tilde{B}$. The part $\sigma \geq 1/2$ is treated similarly. If χ is replaced by $1-\chi$ then the result is rapidly decaying as $t \to 0$, as can easily be seen from the rapid decay of $B(1-\chi)$ as $s \to 0$.

Formula (16) follows immediately from (18).

Similar arguments also show smoothness and rapid decay of $A * B$ for $x \neq y$. □

The following is the central calculation for the whole heat kernel construction, and the reader should try to do it herself before (or instead of) reading the proof.

Proposition 2.7. (1) *Let $A \in \Psi_H^\alpha(M)$, $\alpha \leq -1$. Then $(\partial_t - \Delta_x)A \in \Psi_H^{\alpha+1}(M)$.*
(2) *If $a = \Phi_\alpha(A)$ and $r = \Phi_{\alpha+1}((\partial_t - \Delta_x)A)$ then*

$$r(X,y) = \left[-\frac{n+2}{2} - \alpha - \frac{1}{2}X\partial_X - \Delta_X^{0,y}\right] a(X,y). \tag{19}$$

Here, $X\partial_X := \sum_i X_i \partial_{X_i}$, and $\Delta_X^{0,y} = \sum_{ij} g^{ij}(y)\partial_{X_i}\partial_{X_j}$ is the leading part of the Laplacian, with coefficients frozen at y, acting in X.

We will only use a consequence of (19): When computing the leading term of $(\partial_t - \Delta_x)A$ at y one may forget the lower order part of the Laplacian, the x-dependence in its leading term, and the t-dependence of $\tilde{A}$.

Proof. Write $A(t,x,y) = t^{-l}\tilde{A}(t, \frac{x-y}{\sqrt{t}}, y)$, $l = \frac{n+2}{2} + \alpha$. We have

$$\begin{aligned} \partial_t A &= -l\,t^{-l-1}\tilde{A} - t^{-l}\frac{x-y}{2t^{3/2}}\partial_X F + t^{-l}\partial_t \tilde{A} \\ &= t^{-l-1}(-l - \frac{1}{2}X\partial_X)F + R_1, \end{aligned}$$

and R_1 is in $\Psi_H^{\alpha+1/2}(M)$ since $\partial_t = \frac{1}{2\sqrt{t}}\partial_{\sqrt{t}}$.

Next, $\partial_{x_i}(t^{-l}\tilde{A}) = t^{-l-1/2}\partial_{X_i}\tilde{A}$, and this gives

$$\begin{aligned}\Delta_x A &= t^{-l-1}\sum_{i,j} g^{ij}(x)\partial_{X_i}\partial_{X_j}\tilde{A} + t^{-l-1/2}\sum_i b_i(x)\partial_{X_i}\tilde{A}\\ &= t^{-l-1}\sum_{i,j} g^{ij}(y)\partial_{X_1}\partial_{X_2}\tilde{A} + R_2.\end{aligned}$$

The remainder R_2 arises from two sources: First, we Taylor expand $g^{ij}(x) = g^{ij}(y) + h^{ij}(x,y)(x-y)$, with smooth matrix-valued h^{ij}, and rewrite the second term as $\sqrt{t}h^{ij}(y+X\sqrt{t},y)X$. Second, it contains the lower order part of Δ_x, where we rewrite $b_i(x) = b_i(y+X\sqrt{t})$. This shows that $R_2 \in \Psi_H^{\alpha+1/2}$, in particular it does not contribute to the leading term. Putting these together we obtain the Proposition. ∎

2.2.5. *Evaluation at* $t=0$. In order to deal with the initial condition, we need:

Lemma 2.8. (a) *Let* $A \in \Psi_H^{-1}(M)$ *and* $f \in C^\infty(M)$. *Then* Af, *defined by* $Af(t,x) = \int_M A(t,x,y)f(y)\,dy$, *is in* $C^\infty([0,\infty)_{\sqrt{t}} \times M)$, *and*

$$Af(0,x) = f(x)\int_{T_xM}\Phi_{-1}(A)(X,x)\,dX. \tag{20}$$

(b) *If* $A \in \Psi_H^\alpha(M)$, $\alpha < -1$, *then* $Af(0,x) = 0$.

The measure on T_xM in (20) is the one coming from the scalar product $g(x)$.

Proof. (a) It is clear that, for $t \to 0$, only points y near x contribute. So we can write, with a cutoff χ supported in a coordinate patch around x, and equal to one near x,

$$\begin{aligned}Af(0,x) &= \lim_{t\to 0+} t^{-n/2}\int_{\mathbb{R}^n}\tilde{A}(t,\frac{x-y}{\sqrt{t}},y)f(y)\chi(y)\,dy\\ &= \lim_{t\to 0+}\int_{\mathbb{R}^n}\tilde{A}(t,X,x-X\sqrt{t})f(x-X\sqrt{t})\chi(x-X\sqrt{t})\,dX,\end{aligned}$$

and this equals (20) since the limit can be put inside the integral by the dominated convergence theorem.

(b) Write $A = t^{-\alpha-1}B$, $B \in \Psi_H^{-1}$, and use (a). ∎

2.3. **The Volterra series.** It is one of the convenient features of the heat equation that there is a very simple procedure to obtain an exact solution from a parametrix.

We first state 'Duhamel's principle' which shows how the convolution product arises:

Lemma 2.9. *Suppose* $K_1 \in \Psi_H^{-1}$ *satisfies* (5), *and* $S \in \Psi_H^\beta$ *with* $\beta < 0$. *Then*

$$\begin{aligned}&(\partial_t - \Delta_x)(K_1 * S) = S + R * S,\\ &\lim_{t\to 0+} K_1 * S = 0.\end{aligned} \tag{21}$$

Proof. Formally, this is easy: Just apply the formula $\partial_t \int_0^t h(t,s)\,dt = h(t,t) + \int_0^t \partial_t h(t,s)\,ds$ to the integral defining $K_1 * S$ and put the Δ_x under the integral sign.

Really, one should be a little careful about convergence, interchanging differentiation and integration and such things. This is left as an exercise. [15] The initial condition follows from Lemma 2.8(b). □

In particular, for $R = 0$ this says: From a solution of the initial value problem (1), with the homogeneous equation, one may obtain a solution of the inhomogeneous equation, with zero initial condition, using the convolution product. The advantage of translating to the latter problem here is that an operator of the form (Identity plus small) may be inverted explicitly using the 'geometric series', which in this context is sometimes called the Volterra series.[16]

Denote $R^{*N} = R * R * \cdots * R$, with N factors.

Proposition 2.10. *Assume $K_1 \in \Psi_H^{-1}$ satisfies* (5) *with $R \in \Psi_H^{-1/2}$.*

(a) *Then*

$$K := K_1 - K_1 * R + K_1 * R * R - \dots \tag{22}$$

converges in $C^\infty((0,\infty) \times M^2)$, and $K \in \Psi_H^{-1}(M)$.

(b) *K is a heat kernel, that is, it satisfies* (1).

(c) *The series* (22) *is an asymptotic series as $t \to 0$. More precisely, $K_1 * R^{*N} \in \Psi_H^{-1-N/2}(M)$.*

Proof. (c) is obvious from the composition theorem, Proposition 2.6, and (b) is clear once convergence is proven, since Duhamel's principle gives $(\partial_t - \Delta_x)(K_1 * R^{*m}) = R^{*m} + R^{*(m+1)}$, so the sum telescopes. Also, the initial condition is not affected by the terms involving R, by Lemma 2.8(b).

Let us show uniform convergence first: Let $S = R^{*N}$, for a fixed $N \geq n/2 + 1$. Then $S \in \Psi_H^{-n/2-1}$, so S is bounded for bounded t. This gives

$$\begin{aligned} S^{*m}(t,x,y) = \int_{0 \leq t_1 \leq \dots \leq t_{m-1} \leq t} \int_{M^{m-1}} S(t-t_1,x,z_1) S(t_1-t_2,z_1,z_2) \dots \\ \dots S(t_{m-2}-t_{m-1},z_{m-2},z_{m-1}) S(t_{m-1},z_{m-1},y)\, dz_1 \dots dz_{m-1}\, dt_1 \dots dt_{m-1}. \end{aligned} \tag{23}$$

The integrand is bounded by C^m, if C is an upper bound for $|S|$ on $(0,t) \times M^2$, the volume of the domain of integration in the z_i-variables is $(\operatorname{vol} M)^{m-1}$, and the volume in the t_i-variables is $t^{m-1}/(m-1)!$, so we get

$$|S^{*m}(t,x,y)| \leq \frac{t^{m-1} (\operatorname{vol} M)^{m-1} C^m}{(m-1)!}.$$

Clearly, then, $|K_1 * R^{i+mN}|$ has the same bound for $i = N, \dots, 2N-1$ and $m = 1, 2, 3, \dots$, and this proves convergence in C^0. Similar estimates hold with l derivatives, for any fixed l, if N is chosen as $n/2 + 1 + l$ instead. This proves convergence in C^∞. To show $K \in \Psi_H^{-1}$, note that we have, from the estimates

[15] Note that part of the statement is that $R * S$ makes sense. This does not follow from Proposition 2.6 since $R \in \Psi_H^0$ only! (We are not assuming anything about the form of K_1, although this generality is not needed here.) A more careful analysis shows that $R * S$ is defined for $R \in \Psi_H^0$ if $\int_{\mathbb{R}^n} \tilde{R}(0,X,y)\, dX = 0$ for each y, and that this is satisfied for R arising as derivative.

[16] In [12], this is called Levi's sum. A Volterra series is very similar to a Neumann series; both invert an operator $I - R$ as $I + R + R^2 + \dots$. But for the Neumann series one ascertains convergence by assuming the norm of R to be less than one (in a suitably chosen space). For the Volterra series no norm estimate is needed, the convergence follows rather from a sort of 'negative order' and 'Volterra' (i.e., the integral kernel vanishes above the diagonal) condition on R.

just proven, that for any l and N there is $K_N \in \Psi_H^{-1}$ with $K = K_N + O(t^N)$ in C^l. Clearly, this gives (a) and (b) in Definition 2.1. If one sets $\tilde{K}(t,X,y) = t^{n/2}K(t, y + X\sqrt{t}, y)\chi(y + X\sqrt{t}) = \tilde{K}_N(t,X,y) + O(t^{N+n/2})\chi(y + X\sqrt{t})$, with a cutoff function χ supported near y, then $X \le Ct^{-1/2}$ on the support of χ, so one gets (c) also. □

2.4. **Proof of the Theorem of Minakshisundaram-Pleijel.**

2.4.1. *Existence of a heat kernel in* $\Psi_H^{-1}(M)$. By Lemma 2.4(b), we can find $K_1 \in \Psi_H^{-1}$ with leading term $(X,y) \mapsto (4\pi)^{-n/2}e^{-|X|^2_{g(y)}/4}$ (one choice for this is (7)). By Lemma 2.8(a), this satisfies the initial condition in (5). Next, by Proposition 2.7 and the remark following it[17] $R := (\partial_t - \Delta_x)K_1$ is in Ψ_H^0 with leading term $\Phi_0(R) = 0$, so actually $R \in \Psi_H^{-1/2}$ by Lemma 2.4(a). Therefore, the Volterra series, Proposition 2.10, gives a heat kernel.

2.4.2. *Locality of the heat kernel coefficients.* Instead of the leading term of $A \in \Psi_H^\alpha(M)$ one can consider the leading l-jet for $l \ge 0$; locally, this is given by the first l terms of the Taylor expansion of $\tilde{A}(t,X,y)$ at $\sqrt{t} = 0$. (It is harder to define this invariantly, but not important here.) Then it is clear from (18) that the leading l-jet of $A * B$ is determined (explicitly, bilinearly) by the leading l-jets of A and B. (Of course, it would be easy to be more precise here.) The leading l-jet of K_1 at (X,y) is of the form $p(X,y)e^{-|X|^2_{g(y)}/4}$ with p a polynomial in X of degree $2l$ whose coefficients are derivatives of g up to order l, taken at y. Since only finitely many terms in the Volterra series contribute to a given jet order of K, it follows that the l-jet of $K(t,x,x)$ is determined by finitely many derivatives of g at x.

2.4.3. *Only integral powers of t appear in the heat trace asymptotics.* Call an element $K \in \Psi_H^\alpha(M)$, $\alpha \in -\mathbb{N}_0/2$, *even* if the following is true: If

$$\tilde{K}(t,X,y) \sim \sum_{j=0}^{\infty} k_j(X,y)t^{j/2} \tag{24}$$

is the Taylor series for $\tilde{K}$ (defined in (9)) at $t = 0$ then k_j is even in X if $j/2+\alpha \in \mathbb{Z}$, and odd otherwise[18]. This condition is independent of the choice of coordinates since in (14) $\sqrt{t}$ only occurs in the combination $X\sqrt{t}$.

Furthermore, it is clear that ∂_t and ∂_{x_i} and multiplication by smooth functions of x map even elements to even elements, and that the convolution of even elements is even. Also, the leading term of K_1 is even, so clearly K_1 can be chosen even.

Therefore, the heat kernel constructed above is even. In particular, $k_j(0,y) = 0$ for j odd. This proves Theorem 1.1.

Note that we have proved more than Theorem 1.1, since we also have information on K for $x \ne y$.

2.4.4. *Uniqueness.* For a nice argument using duality, see [13], page 271.

2.5. **More remarks: Formulas, generalizations etc.**

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[17] In fact, if one hadn't 'guessed' K_1, one could easily derive it from solving $[-n/2 - 1/2X\partial_X - \Delta_X^{0,y}]F(X,y) = 0$, for any fixed y, using the Fourier transform in X. This has a unique Schwartz solution, up to a constant factor which can be determined from the initial condition.

[18] Even: $k_j(-X,y) = k_j(X,y)$; odd: $k_j(-X,y) = -k_j(X,y)$.

2.5.1. *Recursion instead of Volterra series.* Instead of using the Volterra series right from the beginning, one may proceed recursively to obtain a parametrix to any order, as follows:

Determine successively $K_i \in \Psi_H^{-1}$, $i = 1, 2, \ldots$, with $R_i := (\partial_t - \Delta_x)K_i \in \Psi_H^{-i/2}$, as follows: Determine K_1 as before, so that $R_1 \in \Psi_H^{-1/2}$. Then suppose we have obtained K_i so that $R_i \in \Psi_H^{-i/2}$. We then wish to determine T_i of suitable order so that $K_{i+1} := K_i + T_i$ satisfies $R_{i+1} \in \Psi_H^{-(i+1)/2}$ where $R_{i+1} = R_i + (\partial_t - \Delta_x)T_i$. Since R_i is only in $\Psi_H^{-i/2}$, we require $T_i \in \Psi_H^{-i/2-1}$ and to be chosen such that $\Phi_{-i/2}(R_{i+1})$ vanishes. By Proposition 2.7 this is equivalent to

$$(-\frac{n+2}{2} + \frac{i}{2} - \frac{1}{2}X\partial_X - \Delta_X^{0,y})F_i(X, y) = -\Phi_{-i/2}(R_i) \tag{25}$$

for the leading term F_i of T_i. This can easily be solved using the Fourier transform (see [13], page 268). Alternatively, one may translate it back to an inhomogeneous heat equation on $\mathbb{R}^n$, with constant coefficients, and solve this using the standard heat kernel and Duhamel's principle.

This gives a parametrix to any order, and then the standard Volterra series (with bounded remainder) may be used to get rid of the error term.

2.5.2. *Analogies to the standard pseudodifferential calculus.* The essential properties of the spaces $\Psi_H^\alpha(M)$ which were used in the proof are also the standard properties of the pseudodifferential calculus:

- The Ψ_H^α, $\alpha \in -\mathbb{N}/2$, form a *filtered algebra*, that is $\Psi_H^{-1/2} \supset \Psi_H^{-1} \supset \ldots$ and $\Psi_H^\alpha * \Psi_H^\beta \subset \Psi_H^{\alpha+\beta}$.
- One has a notion of 'leading term'. This corresponds to the principal symbol in the pseudodifferential calculus.
- One has a short exact sequence connecting the filtration and the symbol map.

Here one could also include the principle of asymptotic summation. We avoided this since the Volterra series already converges in the usual sense.

We did not introduce operators of positive order in the heat calculus. This would be possible, and then Propositions 2.6 and 2.7 would be special cases of one composition formula, but at the expense of having to deal with distributions. (Not really a problem, but also nice to avoid.)

2.5.3. *Calculation of the coefficients.* It is clear from an inspection of the proof that the coefficients $a_i(x)$ are determined polynomially by the g_{ij} and their derivatives at x. It is of interest, especially in view of the inverse spectral problem, to find these expressions explicitly, or have some systematic understanding of them. There are various ways of doing this:[19]

(1) Simply evaluate the Volterra series. Say you want to find the $a_j(0)$ in a fixed coordinate system. For this, simply replace all x, y, z variables by $x = \sqrt{t}\xi$, $y = \sqrt{t}\eta$, $z = \sqrt{t}\zeta$; Taylor develop K_1 in (7) with respect to $\sqrt{t}$ around $t = 0$, this gives

$$K_1(t, x, y) \sim t^{-n/2} \sum_{k=0}^{\infty} p_k(\xi, \eta) t^{k/2} e^{-|\xi-\eta|^2/4},$$

[19]Though I am quite sure that the last word has not been spoken on this problem!

if $g_{ij}(0)=\delta_{ij}$, say, with polynomials p_k of degree $2k$. A similar formula will hold for $R=(\partial_t-\Delta_x)K_1=-(\sum_{ij}(g^{ij}(x)-g^{ij}(y))\partial_{x_i}\partial_{x_j}+\sum_i b_i(x)\partial_{x_i})K_1$, with the power $t^{-n/2-1/2}$ in front. Putting this into the convolution product $K_1 * R^{*(m-1)}$ (compare (23)), setting $\tau_i=(t_{i-1}-t_i)/t$, $i=1,\dots,m$ (with $t_0:=t$, $t_m:=0$), and $w_i=\zeta_{i-1}-\zeta_i$ (with $\zeta_0=\zeta_m=0$), one gets an explicit linear combination of polynomials in the g_{ij}, g^{ij} and their derivatives whose coefficients are of the form

$$\int_\Sigma \int_H \sigma^\gamma \prod_{i=1}^m (W_i^{\delta_i} e^{-|W_i|^2/4\sigma_i})\, dW d\sigma$$

where $\Sigma=\{(\sigma_1,\dots,\sigma_m): \sigma_i\geq 0, \sum_i \sigma_i=1\}$ and $W=\{(W_1,\dots,W_m): W_i\in\mathbb{R}^n, \sum_i W_i=0\}$ and $\gamma\in(\mathbb{Z}/2)^m$, $\delta_i\in\mathbb{N}_0^n$ are multi-indices. The W-integral is just a multiple convolution evaluated at zero and can be evaluated to be $(\sum_i \sigma_i)^{-n/2}$ times a polynomial in the $\sqrt{\sigma_i}$, for example by use of Fourier transform. Then the σ-integral can easily be evaluated in terms of the Gamma function.

(2) Recall that only the leading term of K_1 was determined, so one might try a different K_1 with the same leading term. Instead of (7) one may try the more geometric $K_1^{\text{geom}}(t,x,y)=(4\pi t)^{-n/2}e^{-\operatorname{dist}(x,y)^2/4t}$, where dist is the Riemannian distance function. This turns out to be better since then R is of order -1 instead of only $-1/2$. Then the integrality of t-powers in the expansion is clear from the start, and the calculations become shorter.

Also, one may find K by making the ansatz

$$K(t,x,y)\sim K_1^{\text{geom}}(t,x,y)(b_0(x,y)+tb_1(x,y)+t^2b_2(x,y)+\dots),$$

plugging this into the heat equation and solving recursively for the b_j (in normal polar coordinates).[20]

(3) The coefficients may sometimes be found using invariant theory. This works as follows: First, a careful look at the recursions (or the Volterra series) shows how many factors and derivatives of the metric can occur in a_i. Next, a_i is given by a polynomial expression in these derivatives, and the resulting number must be the same no matter which coordinate system was chosen to begin with. This restricts the set of possible polynomials enormously (to a vector space of quite low dimensions, for small i), and reduces the problem to the calculation of a few undetermined coefficients. These may then be determined by explicit calculation of some example manifolds (since they are universal, i.e. independent of the manifold). See [6], for example.

(4) In the heat equation approach to the Index Theorem one needs to compute the $a_{n/2}$-term (i.e. the coefficient of t^0), not for the Laplacian on functions, but for a 'generalized Laplacian' (arising from certain Dirac operators), for which the asymptotics still holds. From what was said above, the computation of this seems exceedingly hard unless n is small, but a careful analysis allows to extract the information that is needed by an additional scaling argument, for any n. See [2], [13].

(5) There are amazing explicit formulas found by Polterovich [14] and later simplified (both the formula and the proof, which fits on a few lines) and

[20] This is sometimes called the Hadamard parametrix in the mathematical literature, and the De Witt expansion in the physics literature, see [1],[2],[4], [5], for example.

generalized by Weingart [15]:

$$a_k(y) = \sum_{l=0}^{k} \left(-\tfrac{1}{4}\right)^l \binom{k+\frac{n}{2}}{k-l} \left[\frac{(-1)^{k+l}}{(k+l)!} \Delta_x^{k+l} \left(\frac{1}{l!} \operatorname{dist}^{2l}(x,y) \right) \right]_{|x=y} .$$

(6) There are other approaches to the computation. See for example the book [10], which also contains many examples.

2.5.4. *Generalization to other elliptic operators.* If the Laplacian is replaced by any elliptic differential operator P, of order $d > 0$, acting on a vector bundle, essentially the same procedure works to show the existence and uniqueness of a corresponding 'heat kernel', as long as the 'model solutions' (generalizing (6)) are rapidly decaying off the diagonal. Since these can be obtained using Fourier transform from the leading part of P, with coefficients frozen at y, this translates to a condition on the principal symbol of P [21]. The minor adjustments are: $\sqrt{t}$ should be replaced by $t^{1/d}$ everywhere. K takes values in homomorphisms from the fiber over y to the fiber over x, so the leading term has values in Endomorphisms of the fiber over y. In the uniqueness argument, the dual operator must be used.

[21]The condition is that all eigenvalues of the principal symbol (which takes values in endomorphisms of the bundle) have negative real part; sometimes this is called Petrovski-ellipticity.

3. Manifolds with boundary

Our next goal is to prove an analogue of Theorem 1.1 for the case of a compact manifold with boundary. We will impose Dirichlet boundary conditions; other boundary conditions (Robin, Neumann) could be treated in the same way.

Because of the local nature of the heat kernel at small times one expects, and it is indeed the case, that at any interior point the expansion (2) still holds. The new phenomenon is that the expansion does not hold uniformly as x approaches the boundary. This is not just a matter of being pedantic. It has a very tangible consequence: The asymptotics of the heat trace, $\int_M K(t,x,x)\,dx$, now has terms of the form $t^{-n/2+j/2}$ for *each* $j \in \mathbb{N}_0$, not just for even j.

We will derive this from a detailed analysis of the heat kernel uniformly near the boundary.

In particular, we will prove:

Theorem 3.1. *Let M be a compact Riemannian manifold with boundary. Then there is a unique Dirichlet heat kernel, that is, a function*

$$K \in C^\infty((0,\infty) \times M \times M)$$

satisfying

$$\begin{aligned} (\partial_t - \Delta_x) K(t,x,y) &= 0, \\ K(t,x,y) &= 0 \quad \textit{whenever } x \in \partial M, \\ \lim_{t\to 0+} K(t,x,y) &= \delta_y(x). \end{aligned} \tag{26}$$

The smoothness of $K(t,x,x)$ as $t \to 0$ may be described as follows:

$$K(t,x,x) = t^{-n/2}\,(A(t,x) + B(t,x)) \tag{27}$$

with $A \in C^\infty([0,\infty) \times M)$ and B supported near the boundary, where in local coordinates $(x', x_n) \in U' \times [0,\epsilon) \subset M$, $U' \subset \mathbb{R}^{n-1}$ open, one has

$$B(t,x) = b(t, x', x_n/\sqrt{t}), \quad b \in C^\infty([0,\infty)_{\sqrt{t}} \times U' \times \mathbb{R}_+) \tag{28}$$

with $b(t,x',\xi_n)$ rapidly decaying as $\xi_n \to \infty$.

We use the notation $[0,\infty)$ for the time interval, while $\mathbb{R}_+$, which is also $[0,\infty)$, is used for the spacial variable x_n.

Note that M^2, $[0,\infty) \times M$ and $[0,\infty) \times U' \times \mathbb{R}_+$ are manifolds with corners, i.e. locally of the form $\mathbb{R}^k_+ \times \mathbb{R}^l$ (with $k \leq 2$ here). By definition, a function on $\mathbb{R}^k_+ \times \mathbb{R}^l$ is *smooth* if it can be extended smoothly to a neighborhood of this set in $\mathbb{R}^{k+l}$. This is easily seen to be invariant under diffeomorphisms of $\mathbb{R}^{k+l}$ that preserve $\mathbb{R}^k_+ \times \mathbb{R}^l$ and is therefore well-defined on a manifold with corners.

Note that, by the rapid decay of B, (27) and the smoothness of A give the 'old' asymptotic expansion of $K(t,x,x)$ for x a fixed interior point (simply take the Taylor series of A around $t = 0$). In fact, the Taylor coefficients of A at $t = 0$ are given by the same polynomial expressions in the metric coefficients and their derivatives as in the case without boundary.

We will actually prove more: We will describe the behavior of K not only on the diagonal, but also nearby, in a similar manner as was done in the case without boundary.

Corollary 3.2. *The heat trace has an asymptotic expansion*[22]

$$\int_M K(t,x,x)\,dx \sim t^{-n/2}\left(\alpha_0 + \alpha_{1/2}t^{1/2} + \alpha_1 t + \dots\right). \tag{29}$$

Our proof of Theorem 3.1 follows the same pattern as that of Theorem 1.1: Starting from homogeneity considerations and decay properties of explicit model solutions, a 'calculus', that is a class of functions expected to contain the heat kernel and its approximations, is constructed. This is shown to be closed under composition and to have a notion of leading term, whose vanishing characterizes an element's being of lower order (i.e. it has a short exact sequence). These properties, together with the model solutions and a simple Volterra series argument, already suffice to construct the heat kernel.

It is remarkable that exactly the same program works in the case with boundary, with only minor details added at most steps, once one has guessed the form of the calculus. The main difference is that now there are two models: At interior points the model is Euclidean space, and at boundary points the model is Euclidean half space. So the main initial effort lies in understanding exactly which functions have the two corresponding model behaviors simultaneously, and how the transition between them works. This also leads to the leading term being a *pair* of functions satisfying a certain compatibility condition. Once this is accomplished, everything is automatic.

Here are a few references for alternative approaches: The Hadamard (= De Witt) Ansatz (see Section 2.5.3(2)) was generalized to the case with boundary in [11]; M. Kac in his famous article [9] gives a nice method for finding the first two coefficients in the case of a plane convex domain. This was refined in [12] to the third coefficient; an interesting observation here was that the Volterra series works also with very low regularity metric, so can be used for the double of a manifold with boundary. A quite different approach uses the technique of boundary layers, see [3] for example. Related is the reduction to the boundary used by Greiner [7], who considers general elliptic differential operators (instead of the Laplacian) and uses pseudodifferential operators. Grubb gives in [8] a systematic study of pseudodifferential boundary value problems (Boutet-de-Monvel's calculus) and proves the heat asymptotics for these.

3.1. **The boundary heat calculus.**

3.1.1. *Motivation.* In the case of manifolds without boundary we were guided by the homogeneity of the heat equation (which suggested looking at functions of $x/\sqrt{t}$), the (approximate) translation invariance of the initial condition (which suggested looking at functions of $(x-y)/\sqrt{t}$ instead), and the exponential decay of the model, i.e. the Euclidean heat kernel on $\mathbb{R}^n$. The definition of the heat calculus reflected precisely these ideas.

What is new in the case of a manifold with boundary? The only really new point is that the boundary condition breaks part of the translation invariance: For points 'very near' the boundary, one has translation invariance only in directions tangent

[22]For the proof it suffices to consider the integral $\int B(t,x)\chi(x)\,dx$ for a smooth cutoff function χ supported in a coordinate patch where (28) is valid. Introducing the new variable $\xi_n = x_n/\sqrt{t}$ one sees that this equals $\sqrt{t}\int_{\mathbb{R}^{n-1}\times\mathbb{R}_+} b(t,x',\xi_n)\chi(x',\xi_n\sqrt{t})\,dx'd\xi_n$ which clearly converges and is smooth in $\sqrt{t}$ by the smoothness and rapid decay of b.

to the boundary. This means that, at least near the boundary, we should expect the heat kernel to be a function of t, $(x'-y')/\sqrt{t}$, $x_n/\sqrt{t}$ and $y_n/\sqrt{t}$ and y', where here and always we use coordinates near the boundary

$$(x', x_n) \in U = U' \times [0, \epsilon) \subset M, \quad U' \times \{0\} = U \cap \partial M, \quad U' \subset \mathbb{R}^{n-1}. \tag{30}$$

This expectation is supported by the explicit formula for the Dirichlet heat kernel on the Euclidean half space $\mathbb{R}^{n-1} \times \mathbb{R}_+$:

$$E_\partial(t, x, y) = (4\pi t)^{-n/2} \left(e^{-|x-y|^2/4t} - e^{-|x^*-y|^2/4t} \right), \quad x^* := (x', -x_n), \tag{31}$$

which may be rewritten

$$E_\partial(t, x, y) = (4\pi t)^{-n/2} e^{-|X'|^2/4} \left(e^{-(\xi_n-\eta_n)^2/4} - e^{-(\xi_n+\eta_n)^2/4} \right) \tag{32}$$

where

$$X' = \frac{x'-y'}{\sqrt{t}}, \quad \xi_n = \frac{x_n}{\sqrt{t}}, \quad \eta_n = \frac{y_n}{\sqrt{t}}. \tag{33}$$

Apart from this new feature, we would like to proceed essentially as in the case without boundary. That is, we would like to define a class of functions on $(0, \infty) \times M^2$, to be called the boundary heat calculus, which:

- reflects the homogeneity and decay properties of the model heat kernels on $\mathbb{R}^{n-1} \times \mathbb{R}_+$ and on $\mathbb{R}^n$,
- has a notion of 'order',
- has a notion of leading part, with a corresponding short exact sequence, and
- has a composition theorem.

One way to look at (31) is this: E_∂ is the sum of a 'direct' term, which equals the $\mathbb{R}^n$ heat kernel E, and a reflected term. The reflected term is chosen to satisfy the heat equation (with zero initial condition) and with boundary data precisely cancelling the restriction of the direct term to the boundary. From the principle of locality it is to be expected, and can be read off from formula (32), that the reflected term decays rapidly on the scale of $\sqrt{t}$ as x or y leaves the boundary. In particular, E_∂ reduces to E plus $O(t^\infty)$ as soon as either x or y stays away a fixed distance from the boundary.

In addition to this we will need to look at E_∂ as *one* basic object, rather than as the difference of two. This is imposed on us by our method: Only this allows for a reasonable notion of leading part. Also, it is motivated by the homogeneity considerations above[23].

This motivates the following definition.

3.1.2. *Definition of the calculus.*

Definition 3.3. *Let M be a manifold with boundary. The boundary heat calculus, denoted $\Psi^\alpha_{H,\partial}(M)$, is, for each $\alpha \leq 0$, the space of functions A on $(0, \infty) \times M^2$ satisfying properties (a), (b) of Definition 2.1, property (c) for interior points p, and in addition:*

[23] and by the expectation that only this changed perspective allows generalization to other geometries, for example conical singularities where the reflection principle is not available.

(d) *for each* $p \in \partial M$ *there is a coordinate neighborhood as in* (30) *and functions*

$$\tilde{A}^{dir} \in C^\infty([0,\infty)_{\sqrt{t}} \times \mathbb{R}^n \times U) \tag{34}$$

$$\tilde{A}^{refl}, \tilde{A}^{bd} \in C^\infty([0,\infty)_{\sqrt{t}} \times \mathbb{R}^{n-1} \times \mathbb{R}^2_+ \times U') \tag{35}$$

so that for $x, y \in U$, $t > 0$ *one has*

$$\begin{aligned} A(t,x,y) &= t^{-\frac{n+2}{2}-\alpha}\left(\tilde{A}^{dir}(t, \frac{x-y}{\sqrt{t}}, y) - \tilde{A}^{refl}(t, \frac{x'-y'}{\sqrt{t}}, \frac{x_n}{\sqrt{t}}, \frac{y_n}{\sqrt{t}}, y')\right), \\ &=: t^{-\frac{n+2}{2}-\alpha}\tilde{A}^{bd}(t, \frac{x'-y'}{\sqrt{t}}, \frac{x_n}{\sqrt{t}}, \frac{y_n}{\sqrt{t}}, y') \end{aligned} \tag{36}$$

with rapid decay for $\tilde{A}^{dir}$ *as in* (10) *and*

$$\tilde{A}^{refl}(t, X', \xi_n, \eta_n, y') = O((\xi_n + \eta_n + |X'|)^{-\infty}), \tag{37}$$

together with all derivatives, uniformly for bounded t.

Note that $\tilde{A}^{\text{refl}}$ depends on the same number of variables as $\tilde{A}^{\text{dir}}$ (and as A), as it should.

One may be tempted to include the boundary condition in the calculus ($A(t,x,y) = 0$ whenever $x \in \partial M$), but this is not a good idea since applying Δ_x would get us out of the calculus.

Let us check that (d) implies (c) for y near an interior point of U: Simply set $\tilde{A}(t,X,y) = \tilde{A}^{\text{dir}}(t,X,y) - \tilde{A}^{\text{refl}}(t, X', X_n + y_n/\sqrt{t}, y_n/\sqrt{t}, y')$, then (36) is exactly (9), and smoothness at $\sqrt{t} = 0$ follows from $y_n > 0$ and (37). Also, one sees that

$$\tilde{A} = \tilde{A}^{\text{dir}} \quad \text{for } t = 0, y_n > 0. \tag{38}$$

For future reference let us rewrite the second equality of (36) in rescaled coordinates:

$$\tilde{A}^{\text{bd}}(t, X', \xi_n, \eta_n, y') = \tilde{A}^{\text{dir}}(t, X', \xi_n - \eta_n, y', \eta_n\sqrt{t}) - \tilde{A}^{\text{refl}}(t, X', \xi_n, \eta_n, y'). \tag{39}$$

We need to define the 'leading term'. Recall that this must be done so that the vanishing of the leading term of an element of $\Psi^\alpha_{H,\partial}$ characterizes its being in $\Psi^{\alpha-1/2}_{H,\partial}$.

Looking at (36), we are led to:

Definition 3.4. *Let* $A \in \Psi^\alpha_{H,\partial}(M)$. *Given coordinates in the interior of* M, *define the* interior leading term, $\Phi^{int}_\alpha(A)$ *just like the leading term in Definition 2.2.*

Given coordinates near the boundary as in Definition 3.3(d), define the boundary leading term, $\Phi^{bd}_\alpha(A)$, *as the function*

$$\Phi^{bd}_\alpha(A)(X', \xi_n, \eta_n, y') = \tilde{A}^{bd}(0, X', \xi_n, \eta_n, y') \quad \textit{for } X' \in \mathbb{R}^{n-1}, \xi_n, \eta_n \in \mathbb{R}_+, y' \in U'. \tag{40}$$

Again, $\tilde{A}^{\text{bd}}$ is not defined uniquely by A, but still its values at $t = 0$ are, as can be seen from simply rearranging (36) into

$$\tilde{A}^{\text{bd}}(t, X', \xi_n, \eta_n, y') = t^{(n+2)/2+\alpha} A(t, y' + X'\sqrt{t}, \xi_n\sqrt{t}, y', \eta_n\sqrt{t}). \tag{41}$$

Again, the highest priority is to analyze how these things depend on the choice of coordinates.

3.1.3. *Coordinate invariance.* We proceed similarly to the boundaryless case. But first we need to define a bundle which will turn out to carry the boundary leading part. Define the vector bundle $E \to \partial M$ with fiber over a point $p \in \partial M$ given by

$$E_p = (T_pM \times T_pM)/T_p\partial M, \text{ where} \tag{42}$$

$$u \in T_p\partial M \text{ acts on } (v,w) \in T_pM \times T_pM \text{ as } (u+v, u+w). \tag{43}$$

(43) makes sense since $T_p\partial M \subset T_pM$ naturally. Note that E_p has dimension $n+1$. One has a vector bundle map defined for $p \in \partial M$ by

$$\beta_p : E_p \to T_pM, \quad [v,w] \mapsto v - w,$$

with $[v,w]$ denoting the equivalence class of the pair (v,w).

Define the inward pointing part of E by

$$E_p^+ = (T_p^+M \times T_p^+M)/T_p\partial M,$$

where $T_p^+M \subset T_pM$ is the closed half space of vectors pointing into the interior of M, or tangent to ∂M. Clearly, this makes sense since $T_p\partial M \subset T_p^+M$, and E_p^+ is a conical subset [24] of E_p. Also, the total space E^+ is a manifold with corners (of codimension two). So the space $C^\infty_{\mathcal{S}(\text{fibers})}(E^+)$ of smooth functions on E^+ which decay rapidly in the fibers is well-defined. Then set

$$\begin{aligned} C^\infty_{\text{bd}}(E^+) := \{\phi^{\text{bd}} \in C^\infty(E^+) : \phi^{\text{bd}} = \beta^*\phi^{\text{dir}} - \phi^{\text{refl}} \text{ for some} \\ \phi^{\text{dir}} \in C^\infty_{\mathcal{S}(\text{fibers})}(T_{\partial M}M), \phi^{\text{refl}} \in C^\infty_{\mathcal{S}(\text{fibers})}(E)\}. \end{aligned} \tag{44}$$

Given local coordinates on M near a boundary point, all of this looks as follows: Let $(\partial_{x_i})_{i=1,\dots,n}$ be the local frame on TM defined by the coordinates, and let $(\partial_{y_i})_{i=1,\dots,n}$ be a second copy of it (so the ∂_{x_i}, ∂_{y_i} are a local frame for $TM \oplus TM$). Then the collection

$$\left(\frac{1}{2}(\partial_{x_i} - \partial_{y_i})\right)_{i=1,\dots,n-1}, \partial_{x_n}, \partial_{y_n}$$

may be taken as frame in E. We denote the corresponding coordinates by $X' = (X_1, \dots, X_{n-1})$, ξ_n, η_n. Clearly, E^+ is characterized by $\xi_n \geq 0$, $\eta_n \geq 0$. With these coordinates on E, and with natural coordinates on TM, one has $\beta(X', \xi_n, \eta_n, y') = (X', \xi_n - \eta_n, y')$. A function ϕ^{bd} on E^+ is in $C^\infty_{\text{bd}}(E^+)$ iff, in coordinates, it is the sum of a function in the variables $X', \xi_n - \eta_n, y'$, rapidly decaying in $(X', \xi_n - \eta_n)$, and a function in X', ξ_n, η_n, y', rapidly decaying in (X', ξ_n, η_n). Roughly speaking, this means that rapid decay is not required when going off to infinity along the 'diagonal' in E^+. This corresponds precisely to the decomposition in (39).

Lemma 3.5. (a) *If condition (d) in Definition 3.3 holds in one coordinate system then it holds in any.*

(b) *The interior leading term $\Phi_\alpha^{int}(A)$ is defined invariantly as a function on the tangent bundle which is smooth up to the boundary and rapidly decaying in the fiber direction:*

$$\Phi_\alpha^{int}(A) \in C^\infty_{\mathcal{S}(\mathit{fibers})}(TM). \tag{45}$$

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[24] that is, $\alpha \in E_p^+$, $r > 0$ imply $r\alpha \in E_p^+$

(c) *The boundary leading term* $\Phi^{bd}_\alpha(A)$ *is defined invariantly as a function on the bundle* $E^+ \to \partial M$ *defined above. Furthermore,*

$$\Phi^{bd}_\alpha(A) \in C^\infty_{bd}(E^+). \tag{46}$$

Proof. (a) Assume $\psi(x) = \bar{x}$, $\psi = (\psi', \psi_n)$ is a coordinate change, and condition (d) holds in the $\bar{x}$-coordinate patch $\bar{U}$, with functions $\bar{\tilde{A}}^{\mathrm{dir}}(t, \bar{X}, \bar{y})$, $\bar{\tilde{A}}^{\mathrm{refl}}(t, \bar{X}', \bar{\xi}_n, \bar{\eta}_n, \bar{y}')$ satisfying the smoothness assumptions (34), (35) and the decay (10), (37). We choose $\tilde{A}^{\mathrm{dir}}$ as in the boundaryless case, see (14), and therefore only need to find $\tilde{A}^{\mathrm{refl}}$ with the same properties as $\bar{\tilde{A}}^{\mathrm{refl}}$, and satisfying

$$\tilde{A}^{\mathrm{refl}}(t, \frac{x'-y'}{\sqrt{t}}, \frac{x_n}{\sqrt{t}}, \frac{y_n}{\sqrt{t}}, y') = \bar{\tilde{A}}^{\mathrm{refl}}(t, \frac{\psi'(x)-\psi'(y)}{\sqrt{t}}, \frac{\psi_n(x)}{\sqrt{t}}, \frac{\psi_n(y)}{\sqrt{t}}, \psi'(y', 0)) \tag{47}$$

for all x, y near p. This works almost the same way as for $\tilde{A}^{\mathrm{dir}}$: We have

$$\psi'(x) - \psi'(y) = h''(x,y)(x'-y') + h'_n(x,y)(x_n - y_n)$$

for a smooth $(n-1)\times(n-1)$ matrix h'' and $(n-1)\times 1$-matrix h'_n, satisfying $h''(y,y) = d'\psi'_y$, $h'_n(y,y) = d_n\psi'_y$. Also, since $\psi_n(x) = 0$ for $x_n = 0$ we have

$$\psi_n(x) = x_n \varphi_n(x)$$

for a smooth function φ_n satisfying $\varphi_n(x', 0) = d_n\psi_{n|(x',0)} > 0$. Then set

$$\tilde{A}^{\mathrm{refl}}(t, X', \xi_n, \eta_n, y') = \bar{\tilde{A}}^{\mathrm{refl}}(t, h''X' + h'_n(\xi_n - \eta_n), \varphi_n(x)\xi_n, \varphi_n(y)\eta_n, \psi'(y', 0))\chi \tag{48}$$

where h'' and h'_n are evaluated at (x, y), and χ is evaluated at x, with $y = (y', \eta_n\sqrt{t})$ and $x = (y' + X'\sqrt{t}, \xi_n\sqrt{t})$. This is clearly equivalent to (47) for x, y near p, and satisfies the required decay.

(b) This is clear as in the boundaryless case. Smoothness up to the boundary follows from (38) and smoothness of $\tilde{A}^{\mathrm{dir}}$ up to the boundary.

(c) Setting $t = 0$ in (48) we get

$$\tilde{A}^{\mathrm{refl}}(0, X', \xi_n, \eta_n, y') = \bar{\tilde{A}}^{\mathrm{refl}}(0, d'\psi'X' + d_n\psi'(\xi_n - \eta_n), d_n\psi_n\xi_n, d_n\psi_n\eta_n, \psi'(y', 0)),$$

with all differentials evaluated at $(y', 0)$, and this is easily seen to be the transformation rule for functions on E, with respect to the coordinates introduced above. The same holds for $\tilde{A}^{\mathrm{dir}}$ by (b), so we are done. ∎

3.1.4. *Short exact sequence.* Before we can state the short exact sequence we need to analyze which function pairs can occur as leading terms. The new aspect here is that there are *compatibility conditions*: It is clear that, in (39), $\tilde{A}^{\mathrm{bd}}$ at $t = 0$ determines $\tilde{A}^{\mathrm{dir}}$ at $t = 0$, $y_n = 0$, for example via $\tilde{A}^{\mathrm{dir}}(0, X', X_n, y', 0) = \lim_{r\to\infty} \tilde{A}^{\mathrm{bd}}(0, X', X_n + r, r, y')$, and this should coincide with the boundary values of the interior leading term.

To put this invariantly, observe that in (44) ϕ^{dir} is determined uniquely by $\phi^{\mathrm{bd}} \in C^\infty_{\mathrm{bd}}(E^+)$ via $\phi^{\mathrm{dir}}(X, p) = \lim_w \phi^{\mathrm{bd}}([X + w, w], p)$, where the limit is over $w \in T^+_p M$ with its class in $T_pM^+/T_p\partial M$ tending to infinity.

Definition 3.6. *The space of leading terms, $C^\infty_{\Phi,\partial}(M)$, is the subspace of $C^\infty_{\mathcal{S}(fibers)}(TM)\times C^\infty_{bd}(E^+)$ given by pairs*[25] (ϕ^{int},ϕ^{bd}) *satisfying*

$$\phi^{int}_{|T_{\partial M}M} = \phi^{dir} \tag{49}$$

where ϕ^{dir} is determined by ϕ^{bd} as explained above.

Lemma 3.7. *The sequence*

$$0 \to \Psi^{\alpha-1/2}_{H,\partial}(M) \to \Psi^{\alpha}_{H,\partial}(M) \xrightarrow{\Phi_\alpha} C^\infty_{\Phi,\partial}(M) \to 0$$

is exact.

Proof. This is clear except possibly at $C^\infty_{\Phi,\partial}(M)$. To prove surjectivity of Φ_α we may clearly work locally near the boundary, so suppose we have functions $\phi^{\rm int}, \phi^{\rm bd} = \beta^*\phi^{\rm dir} - \phi^{\rm refl}$ satisfying (49). Then set, locally,

$$A(t,x,y) = t^{-(n+2)/2-\alpha}\left(\phi^{\rm int}(\frac{x-y}{\sqrt{t}},y) - \phi^{\rm refl}(\frac{x'-y'}{\sqrt{t}},\frac{x_n}{\sqrt{t}},\frac{y_n}{\sqrt{t}},y')\right).$$

This has interior leading part $\phi^{\rm int}$ since $\phi^{\rm refl}$ is rapidly decaying in X', ξ_n, η_n, and has boundary leading part $\phi^{\rm bd}$ because of (49). ∎

3.1.5. *Composition.*

Proposition 3.8. *Let $A\in\Psi^\alpha_{H,\partial}(M)$, $B\in\Psi^\beta_{H,\partial}(M)$, with $\alpha,\beta<0$, and assume M is compact. Then $A*B$ is defined and lies in $\Psi^{\alpha+\beta}_{H,\partial}(M)$. The interior leading term is calculated as in* (16)*, and the boundary leading terms satisfy*

$$\begin{aligned}(a*b)^{bd}(X',\xi_n,\eta_n,p) = \int_0^1\int_{\mathbb{R}^{n-1}}\int_{\mathbb{R}_+}&(1-\sigma)^{-(n+2)/2-\alpha}\sigma^{-(n+2)/2-\beta}\\ &a^{bd}\left(\frac{(X'-Z',\xi_n,\zeta_n)}{\sqrt{1-\sigma}},p\right) b^{bd}\left(\frac{(Z',\zeta_n,\eta_n)}{\sqrt{\sigma}},p\right)d\zeta_n dZ' d\sigma.\end{aligned} \tag{50}$$

(The formula for the leading term will not be used.)

Proof. As in the proof of the case without boundary, it is enough to consider x,y in a coordinate patch U. Furthermore, we may assume that $U=U'\times[0,\varepsilon)$ is a boundary coordinate patch, where A,B have representations as in (36), and to consider the localized integral (17). We replace the integration variables by $\sigma=s/t$, $Z'=(z-y)/\sqrt{t}$, $\zeta_n=z_n/\sqrt{t}$ and introduce new variables $X'=(x'-y')/\sqrt{t}$, $\xi_n=x_n/\sqrt{t}$, $\eta_n/\sqrt{t}$ instead of x'. x_n, y_n. Then (17) becomes $t^{-(n+2)/2-\alpha-\beta}\tilde{C}^{\rm bd}(t,X',\xi_n,\eta_n,y')$ where $\tilde{C}^{\rm bd}(t,X',\xi_n,\eta_n,y')$ equals

$$\int_0^1\int_{\mathbb{R}^{n-1}}\int_{\mathbb{R}_+} d\zeta_n\, dZ'\, d\sigma(1-\sigma)^{-(n+2)/2-\alpha}\sigma^{-(n+2)/2-\beta}. \tag{51}$$

$$\tilde{A}^{\rm bd}(t(1-\sigma),\frac{(X'-Z',\xi_n,\zeta_n)}{\sqrt{1-\sigma}},y'+Z'\sqrt{t})\tilde{B}^{\rm bd}(t\sigma,\frac{(Z',\zeta_n,\eta_n)}{\sqrt{\sigma}},y')\,\chi(y'+Z'\sqrt{t},\xi_n\sqrt{t}).$$

We need to check convergence and rapid decay properties for each of the four terms arising from splitting up $\tilde{A}^{\rm bd}$, $\tilde{B}^{\rm bd}$ as sums of direct and reflected terms (as in (39)). The product of direct terms is done as in the case without boundary.

[25]that the leading term is a pair of functions corresponds to the two symbol levels in the Boutet-de-Monvel calculus, see [8]

We claim that the other three terms are all in $C^\infty_{\mathcal{S}(\text{fibers})}(E^+)$, that is, they decay rapidly in all the variables X', ξ_n, η_n. For example, let us look at the direct term $\tilde{A}^{\text{dir}}$ and the reflected term $\tilde{B}^{\text{refl}}$. In the region $\sigma \leq 1/2$ introduce the variables $W' = Z'/\sqrt{\sigma}$ for Z' and $\rho_n = \zeta_n/\sqrt{\sigma}$ for ζ_n. Then the power of σ is $-1-\beta$, so the integral converges since $\beta < 0$, and the integrand of the $d\rho_n dZ'$ integral is bounded by $(||X'| - |W'|| + |\xi_n - \rho_n|)^{-N}(|W'| + \rho_n + \eta_n/\sqrt{\sigma})^{-N}$ for any N, from which convergence and rapid decay of the integral is easily seen. Derivatives, the region $\sigma \geq 1/2$ and the other cases are treated similarly.

Formula (50) follows immediately from (51). ∎

We also have the analogue of Proposition 2.7:

Proposition 3.9. (1) *Let* $A \in \Psi^\alpha_{H,\partial}(M)$, $\alpha \leq -1$. *Then* $(\partial_t - \Delta_x)A \in \Psi^{\alpha+1}_{H,\partial}(M)$.

(2) *The interior leading terms of* A *and* $R = (\partial_t - \Delta_x)A$ *are related as in* (19), *and the boundary leading terms* $a^{bd} = \Phi^{bd}_\alpha(A)$ *and* $r^{bd} = \Phi^{bd}_{\alpha+1}(R)$ *satisfy*

$$r^{bd}(X', \xi_n, \eta_n, p) = [-\frac{n+2}{2} - \alpha - \frac{1}{2}X'\partial'_X - \frac{1}{2}\xi_n\partial_{\xi_n} - \frac{1}{2}\eta_n\partial_{\eta_n} - \Delta^{0,p}_{X',\xi_n}]a^{bd}(X', \xi_n, \eta_n, p). \tag{52}$$

Here, $\Delta^{0,p}_{X',\xi_n} = \sum_{ij} g^{ij}(p)\partial_{X_i}\partial_{X_j}$ *(with* X_n *replaced by* ξ_n*).*

Again, formula (52) will not be used directly.

Proof. In the interior, this follows from Proposition 2.7. Near a boundary point write $A(t,x,y) = t^{-l}\tilde{A}^{\text{bd}}(t, \frac{x'-y'}{\sqrt{t}}, \frac{x_n}{\sqrt{t}}, \frac{y_n}{\sqrt{t}}, y')$, $l = \frac{n+2}{2} + \alpha$, then the calculation is the same as in the case without boundary, except that X_n is replaced by ξ_n in the formulas, in the t-derivative one has an extra term $-t^{-l}\frac{y_n}{2t^{3/2}}\partial_{\eta_n}\tilde{A}^{\text{bd}} = -t^{-l-1}\frac{1}{2}\eta_n\partial_{\eta_n}\tilde{A}^{\text{bd}}$, and in the computation of $\Delta_x A$ there is an additional contribution to the remainder R_2 from writing $g^{ij}(y) = g^{ij}(y', 0) + h_1^{ij}(y)y_n$, where the second term is $\sqrt{t}\, h_1^{ij}(y', \sqrt{t}\eta_n)\eta_n$ and thus lower order. ∎

3.1.6. *Boundary conditions.* Let

$$\Psi^\alpha_{H,\text{Dir}}(M) = \{A \in \Psi^\alpha_{H,\partial}(M) : A(t,x,y) = 0 \quad \text{whenever } x \in \partial M\}.$$

The following lemma is obvious:

Lemma 3.10. (a) *Let* $A \in \Psi^\alpha_{H,Dir}$, $B \in \Psi^\beta_{H,\partial}$, *where* $\alpha, \beta < 0$. *Then* $A * B \in \Psi^{\alpha+\beta}_{H,Dir}$.

(b) *There is a short exact sequence for* $\Psi^\alpha_{H,Dir}$, *with boundary leading parts vanishing at the 'left' boundary (*$\xi_n = 0$*) of* E^+.

3.1.7. *Evaluation at* $t = 0$. Lemma 2.8 carries over directly, mutatis mutandis; that is, in (20) one uses the interior leading part of A, and the boundary leading part plays no role.

3.2. **The Volterra series.** We restate Proposition 2.10 in the present context:

Proposition 3.11. *Assume $K_1 \in \Psi^{-1}_{H,\partial}$ satisfies*

$$\begin{aligned}(\partial_t - \Delta_x)K_1 &= R \in \Psi^{-1/2}_{H,\partial},\\ K_1(t,x,y) &= 0 \quad \textit{whenever } x \in \partial M, (so K_1 \in \Psi^{-1}_{H,Dir})\\ \lim_{t\to 0+} K_1(t,x,y) &= \delta_y(x).\end{aligned} \tag{53}$$

(a) *Then*

$$K := K_1 - K_1 * R + K_1 * R * R - \dots \tag{54}$$

converges in $C^\infty((0,\infty)\times M^2)$, and $K \in \Psi^{-1}_{H,Dir}(M)$.

(b) *K is a Dirichlet heat kernel, that is, it satisfies* (26)*.*

(c) *The series* (54) *is an asymptotic series as $t \to 0$. More precisely, $K_1 * R^{*N} \in \Psi^{-1-N/2}_{H,Dir}(M)$.*

The proof carries over from Proposition 2.10 with almost no changes. Only in the last sentence in its proof one should use, near the boundary, a cutoff $\chi(x)\chi(y) = \chi(y' + X'\sqrt{t}, \xi_n\sqrt{t})\chi(y', \eta_n\sqrt{t})$ instead, on whose support $|X'| + \xi_n + \eta_n \le Ct^{-1/2}$, which gives the required exponential decay in the reflected term.

3.3. **Construction of the heat kernel.**

Theorem 3.12. *Let M be a compact Riemannian manifold with boundary. Then there is a unique Dirichlet heat kernel K, and it lies in $\Psi^{-1}_{H,\partial}(M)$.*

Furthermore, K may be split $K = K^{int} + K^{bd}$ where $t^{n/2}K^{int}(t,x,x) \in C^\infty([0,\infty)\times M)$ and $K^{bd}(t,x,y) = O([d(x)/\sqrt{t} + d(y)/\sqrt{t}]^{-\infty})$, with $d(x)$ the distance of x to the boundary.

Proof. After all this preparation, this works just the same as in the case without boundary, except that the initial step is modified since there are two models.

Define $(\phi^{\mathrm{int}}, \phi^{\mathrm{bd}}) \in C^\infty_{\Phi,\partial}(M)$ by

$$\begin{aligned}\phi^{\mathrm{int}}(X,p) &= (4\pi)^{n/2} e^{-|X|^2_{g(p)}/4}, \quad p \in M\\ \phi^{\mathrm{bd}}([v,w],p) &= (4\pi)^{n/2}\left(e^{-|v-w|^2_{g(p)}/4} - e^{-|v-w^*|^2_{g(p)}/4}\right), \quad p \in \partial M\end{aligned}$$

where the 'reflected' vector w^* of $w \in T_pM$, for $p \in \partial M$, is defined as follows: Write $w = w_{\mathrm{bd}} + w_n$ with w_{bd} tangential to the boundary and w_n normal to it, with respect to the metric $g(p)$; then $w^* := w_{\mathrm{bd}} - w_n$. [26] With this definition it is clear that $|w| = |w^*|$, so ϕ^{bd} satisfies the boundary condition in Lemma 3.10(b). Also, it is clear that $\phi^{\mathrm{int}}, \phi^{\mathrm{bd}}$ satisfy the compatibility condition (49), so there is $K_1 \in \Psi^{-1}_{H,\mathrm{Dir}}$ with $\Phi_{-1}(K_1) = (\phi^{\mathrm{int}}, \phi^{\mathrm{bd}})$.

[26] A little care is needed here: It would not work to choose *any* boundary adapted coordinates (as before) and then, with $w = (\eta', \eta_n)$, set $w^* = (\eta', -\eta_n)$, since the 'cross terms' in $|v - w*|^2_g$, of the form $g_{in}X_i(\xi_n + \eta_n)$ with $i \le n-1$ would not equal the corresponding terms $g_{in}X_i(\xi_n - \eta_n)$ in $|v-w|^2$ at $\xi_n = 0$, so the boundary condition would be violated by ϕ^{bd} unless $g_{in} = 0$ for all $i \le n-1$. Therefore, only coordinates in which the x_n direction is orthogonal to the tangential directions can be used here, and our definition reflects precisely this, in a coordinate-free way. (Such choice of coordinates, called 'coordinates normal with respect to the boundary' exist, but are not needed here.)

By Proposition 3.9 the remainder $R = (\partial_t - \Delta_x)K_1$ is in $\Psi^0_{H,\partial}$ with leading term[27] $\Phi_0(R) = 0$, so actually $R \in \Psi^{-1/2}_{H,\partial}$, and then the Volterra series gives a heat kernel. Uniqueness can be proved in the same way as before.

Note that $K(t,x,y) = 0$ for $y \in \partial M$ also since this is true for K_1, hence for R, hence for K.

The last claim is clear from the definition of $\Psi_{H,\partial}$, except for the smoothness of $K^{\mathrm{int}}(t,x,x)$ with respect to t (rather than $\sqrt{t}$). The latter follows in the same way as the corresponding statement in the case without boundary, see the discussion after (24). □

[27]again, this could be computed from formula (52), or concluded directly from the fact that this formula says that the leading part can be computed by freezing coefficients and forgetting lower order terms.

References

[1] Marcel Berger, Paul Gauduchon, and Edmond Mazet. *Le spectre d'une variété riemannienne*. Lecture Notes in Mathematics, Vol. 194. Springer-Verlag, Berlin, 1971.

[2] N. Berline, E. Getzler, and M. Vergne. *Heat Kernels and Dirac Operators*, volume 298 of *Grundlehren der mathematischen Wissenschaften*. Springer–Verlag, Berlin, Heidelberg, New York, 1992.

[3] M. Bordag, D. Vassilevich, H. Falomir, and E. M. Santangelo. Multiple reflection expansion and heat kernel coefficients. *Phys. Rev. D (3)*, 64(4):045017, 11, 2001.

[4] Isaac Chavel. *Eigenvalues in Riemannian geometry*, volume 115 of *Pure and Applied Mathematics*. Academic Press Inc., Orlando, FL, 1984. Including a chapter by Burton Randol, With an appendix by Jozef Dodziuk.

[5] Bryce S. DeWitt. *Dynamical theory of groups and fields*. Gordon and Breach Science Publishers, New York, 1965.

[6] Peter B. Gilkey. *Invariance theory, the heat-equation, and the Atiyah-Singer index theorem*. Studies in Advanced Mathematics. CRC Press, Boca Raton, 2 edition, 1995.

[7] Peter Greiner. An asymptotic expansion for the heat equation. *Arch. Rational Mech. Anal.*, 41:163–218, 1971.

[8] Gerd Grubb. *Functional calculus of pseudodifferential boundary problems*, volume 65 of *Progress in Mathematics*. Birkhäuser Boston Inc., Boston, MA, second edition, 1996.

[9] M. Kac. Can one hear the shape of a drum? *Am. Math. Mon., Part II*, 73:1–23, April 1966.

[10] Klaus Kirsten. *Spectral functions in mathematics and physics*. Chapman and Hall/CRC, Boca Raton, Fla., 2002.

[11] D. M. McAvity and H. Osborn. A DeWitt expansion of the heat kernel for manifolds with a boundary. *Classical Quantum Gravity*, 8(4):603–638, 1991. Errata: vol. 9, 1992, p. 317.

[12] H. P. McKean, Jr. and I. M. Singer. Curvature and the eigenvalues of the Laplacian. *J. Differential Geometry*, 1(1):43–69, 1967.

[13] Richard B. Melrose. *The Atiyah-Patodi-Singer index theorem*. A. K. Peters, Ltd., Boston, Mass., 1993.

[14] Iosif Polterovich. Heat invariants of Riemannian manifolds. *Israel J. Math.*, 119:239–252, 2000.

[15] Gregor Weingart. A characterization of the heat kernel coefficients. Preprint, http://arXiv.org/abs/math.DG/0105144, 2001.