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Microlocal heat kernel asymptotics and inverse spectral problems

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MICROLOCAL HEAT KERNEL ASYMPTOTICS AND INVERSE SPECTRAL PROBLEMS.*)
I. Reduction to the Boundary and the Asymptotic Expansion.

Stig I. Andersson, Christian Högfors, Bo Pettersson

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0. Introduction

Given a partial differential operator (PDO), P(x,D) on a manifold M,

$$P(x,D):C^\infty(M) \to C^\infty(M)$$

the most obvious question to ask is what the spectrum, $\sigma(P)$, is. Various aspects of this question are usually called the direct spectral geometry problem. Another possibility is to deduce, inversely, information about the operator P(x,D) assuming $\sigma(P)$ and M are known or to try to construct M from a knowledge of $\sigma(P)$ and P(x,D). These latter problem types constitute the essence of inverse spectral geometry.

This paper will be concerned with two problems. That of reconstructing the geometry and differential topology of M, given à priori (e.g. measured) information about spectral properties of a certain class of PDO's, and a kind of reduction process (via microlocalization).

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The applications we have in mind concern essentially the reconstruction of the shape of bodies from knowledge (mostly inprecise) of their vibration spectra. In the present paper we shall present the mathematical basis and the applications will be the subject of some forthcoming publications.

Mathematically, we shall be dealing with manifolds M having a boundary $\partial M \neq \phi$ (except for Sect. 4) and corresponding boundary value problems for P;

$$P(x,D)u(x) = f(x) \quad \text{in } M$$

$$B_j u(x) = g_j(x) \quad \text{on } \partial M \quad ,$$

$f \in C^\infty(M)$, $g_j \in C^\infty(\partial M)$ given together with the boundary operators

$$B_j : C^\infty(M) \to C^\infty(\partial M) \quad .$$

At the expense of more involved notations, the situation of having sections of vector bundles (i.e. locally vector-valued functions), instead of simply functions, could also be handled. In general one would have to make sure that such a boundary value problem is solvable by imposing conditions of e.g. ellipticity.

Assuming knowledge of the spectrum $\sigma(P)$, it is possible to identify certain spectral invariants, attached to P, with geometric quantities. The way this is done is by considering suitable 1-parameter families of functions of P and to look for the asymptotic behaviour in the parameter.

There are various possible choices for these 1-parameter families of functions of P, but the one we shall use is the θ-function of P,

$$\theta_P(t) := \mathrm{tr}(e^{-tP}) \quad , \quad t>0 \quad .$$

Clearly, not every P(x,D) would make e^{-tP} a trace-class operator, so care has to be exercised in defining $\theta_P(t)$.

As for asymptotic behaviour, one could imagine studying two different kinds of asymptotic behaviour for $\theta_P(t)$, viz. $t \to 0+$ and $t \to +\infty$. Obviously this would correspond to considering very large spectral values and very small spectral values respectively, in view of the fact that for P self-adjoint;

$$\theta_P(t) = \sum_j e^{-t\lambda_j} \quad , \quad \{\lambda_j\} \text{ eigenvalues of } P.$$

In fact, one can show:

$$\lim_{t\to\infty} e^{-tP} = \begin{array}{l}\text{projection operator onto the eigenspace}\\ \text{correponding to the lowest eigenvalue}\end{array}$$

Substantial geometric information is obtained by considering instead the asymptotic expansion for small t, i.e.,

$$\lim_{t\to 0+} \theta_P(t) \quad . \tag{0.1}$$

We shall here demonstrate a new expedient way to derive the form of this asymptotic expansion for suitable classes of operators P(x,D) and suitable boundary conditions.

It is well-known that in considerations involving the t→0+ asymptotics of $\theta_P(t)$ (for say P a differential operator with positive principal symbol), no more information is gained by studying increasingly complex kernels of this type, like e.g.

$$\mathrm{tr}(Q_1(P)e^{-tQ_2(P)}) \tag{0.2}$$

Q_i, i=1,2 polynomials (with positive definite highest order coefficient). It turns out that the asymptotics for (0.2) is essentially given by polynomials in the coefficients of the asymptotic expansion for (0.1).

This paper shall also be concerned with going in the opposit direction. Given P, are there more basic information constituents (obtained by asymptotic expansion), the synthesis of which yields the same information as the asymptotics for (0.1)?

In view of the considerable difficulties involved in computing the expansion coefficents in the asymptotic expansion for (0.1), such a reduction process would be of considerable interest, not only structurally, but also computationally. The possibility of such a reduction is suggested by microlocal analysis.

The interesting situation is that of a manifold with boundary. Since however the microlocal study of boundary problems is poorly developed (c.f. [Mel]), we shall as far as microlocalization is concerned in Section 4, consider only the case of a closed manifold.

A natural framework for $\Theta_P(t)$ is the mixed problem

$$\begin{aligned} &(\frac{\partial}{\partial t} + P_B)\, u(x,t) = 0 \quad , \quad MxR_+ \\ &u(x,0) = u_0(x) \quad , \quad Mx\{0\} \\ &B_j\, u(x,t) = g_j(x,t) \quad , \quad \partial Mx\, R_+ \end{aligned} \tag{0.3}$$

where the domain of $P_B(x,D)$ would naturally be

$$D(P_B) := \{u \in C^\infty(Mx\, R_+) : B_j\, u = g_j \text{ on } \partial Mx\, R_+\}.$$

Formally, the solution to (0.1) would be given by the semigroup:

$$R_+ \ni t \to e^{-tP_B} \quad ,$$

i.e., the object we are interested in.

For nontrivial manifolds M, exact solutions to (0.3) are not available, of course. To construct the asymptotics for $\Theta_P(t)$ it suffices however to have an approximate fundamental solution, a parametrix for the heat equation corresponding to P (in a sense to be made precise shortly) and such objects can be readibly constructed.

Before we proceed to the construction, some general remarks on the underlying strategy for obtaining geometric information out of spectral and analytic data, are appropriate. We shall for elliptic self-adjoint P of second order obtain asymptotic expansions (AE) of the form

$$\lim_{t\to 0+} \Theta_P(t) \sim (4\pi t)^{-n/2} \{ \sum_{j/2 \in N_+}^{\infty} \alpha_j t^{j/2} + \sum_{j \in N_+} \beta_j t^{j/2} \} \tag{0.4}$$

Here, the coefficients $\{\alpha_j\}$ and $\{\beta_j\}$ can be explicitly expressed in terms of the symbol P in M and on ∂M respectively. On the other hand, $\{\alpha_j\}$ and $\{\beta_j\}$ are also expressible in terms of the geometry of M (in case of $\{\alpha_j\}$) and the extrinsic geometry of ∂M (in case of $\{\beta_j\}$), e.g., induced metric on ∂M, second fundamental form.

In fact the coefficients in (0.4) are local Riemannian invariants and can be expressed as (universal) polynomials in terms of the curvature and its covariant derivatives.

Recalling, that for P self-adjoint,

$$\Theta_P(t) = \sum_j e^{-t\lambda_j} = \sum_{\lambda\in\sigma(P)} e^{-t\lambda}\mathrm{mult}(\lambda) \qquad (0.5)$$

($\mathrm{mult}(\lambda)$ = multiplicity of $\lambda\in\sigma(P)$), we have the simple

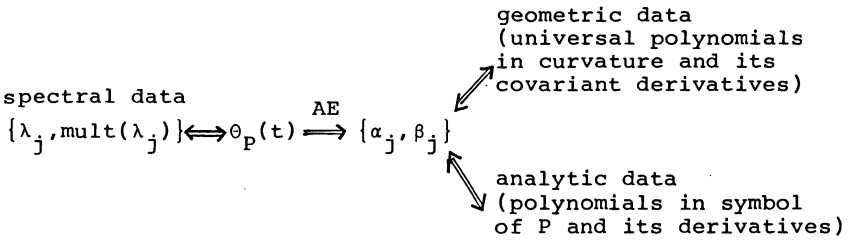
Lemma 0.1: $\Theta_P(t)$ and $\{\lambda_j, \mathrm{mult}(\lambda_j)\}$ determine each other uniquely.

Proof: It suffices to note that (assuming the lowest eigenvalue to be simple)

$$\lim_{t\to\infty} (\Theta_P(t)-1)e^{\mu t} = \begin{cases} 0 & \text{for } \lambda>\mu \\ \mathrm{mult}(\mu) & \text{for } \lambda=\mu \\ \infty & \text{for } \lambda<\mu \end{cases}$$

Remark 0.2: The existence of (0.5) (in the distribution sense), is part of the theory to be presented below.

Since $\Theta_P(t)$ determines $\{\alpha_j, \beta_j\}$ via the AE, we obtain the following situation:



Remark 0.3: Strictly speaking, as will be seen in the precise formulation below, the theory gives us $\{\alpha_j(x), \beta_j(x)\}$ and they are the quantities which should appear in this diagram instead of

$$\alpha_j := \int_M \alpha_j(x)d\mu \quad , \quad \beta_j := \int_{\partial M} \beta_j(x)d\nu \quad .$$

In realistic situations of the kind we have in mind for our applications, one never has complete spectral information but only truncated spectral data:

$$\{\lambda_j, \mathrm{mult}(\lambda_j)\}_{j=0}^{N} \quad , \quad N<\infty$$

To deduce information about the geometry from truncated spectral data requires some extra considerations. This question is in fact related to the question whether there exist operators P such that

the corresponding AE (0.4) breaks off after a finite number of steps, i.e., $\{\alpha_j, \beta_j\}$ all zero for $j>N$. Obviously such a behaviour of the AE can result also from properties of the geometry. If, e.g., $N=1$ it is known that M has to be flat. This question and related problems will be treated in forthcoming publications. As for general references on spectral geometry and heat kernels, we refer to [Giℓ] and [Gr].

1. Parametrices and Reduction to the Boundary

We assume from now on that M is a compact C^∞-manifold of dimension n with C^∞-boundary ∂M. Furthermore, $P(x,D)$ is a second order elliptic operator with positive principal symbol and C^∞-coefficients and B is a C^∞ vector field on ∂M.

We shall be concerned with the mixed problem:

$$\begin{aligned} Lu(x,t) \equiv (\tfrac{\partial}{\partial t} + P(x,D))u(x,t) &= 0 \ , \quad M \times]0,\infty[\\ B\,u(x,t) &= 0 \ , \quad \partial M \times]0,\infty[\\ u(x,0) &= u_0(x) \ , \quad M \times \{0\} \ . \end{aligned} \tag{1.1}$$

The problem (1.1) is local, so by a suitable local change of coordinates we could always work in a chart where;

$$\begin{aligned} M &= \{(x',x_n) \in R^{n-1} \times R \mid x_n>0\} \\ P(x,D) &= -\sum_{j,k=1}^{n} a_{j,k}(x)\, \frac{\partial^2}{\partial x_j \partial x_k} + \sum_{k=1} c_k(x)\, \frac{\partial}{\partial x_k} + d(x) \\ B &= \sum_{k=1}^{n} b_k(x')\, \frac{\partial}{\partial x_k} \end{aligned} \tag{1.2}$$

By the same local change of coordinates we could also achieve that $a_{nj}(x',0) = 0$, $j<n$, which we shall assume from now on. We consider here the localized problem and in Section 3 we shall show how to obtain global information by a partition of unity-argument. So locally we have the mixed problem:

$$\begin{aligned} L\,u(x,t) &= 0 \ , \quad x = (x',x_n) \in R^{n-1} \times R_+ \ , \quad t>0 \\ B\,u(x,t) &= 0 \ , \quad x = (x',0) \ , \quad t>0 \\ u(x,0) &= U_0(x) \ , \quad x = (x',x_n) \in R^{n-1} \times R_+ \ , \quad t=0 \end{aligned} \tag{1.1}_L$$

$L = \frac{\partial}{\partial t} + P$ and B, P given by (1.2).

Def. 1.1: A fundamental solution to $(1.1)_L$ is a function K(x,y,t) on MxMx $]0,\infty[$, C^1 in t and C^2 in x, such that

$$\begin{aligned} L_x K(x,y,t) &= 0 \quad , \quad MxM\times\,]0,\infty[\\ B_x K(x,y,t) &= 0 \quad , \quad \partial M\times M\times]0,\infty[\\ K(x,y,0) &= \delta(x-y) \ , \quad M\times M\times\{0\} \end{aligned} \tag{1.3}$$

Note: Here we write for the sake of brevity M, ∂M instead of the correct local versions of these objects.

Given a fundamental solution, $(1.1)_L$ would be solved by

$$u(x,t) = \int_M K(x,y,t)u_0(y)dy$$

and for the inhomogenous version of $(1.1)_L$, say with Lu=0 replaced by $Lu(x,t) = \phi(x,t)$ on Mx $]0,\infty[$, we would have

$$u(x,t) = \int_M K(x,y,t)u_0(y)dy + \int_0^t ds \int_M K(x,y,t-s)\phi(y,s)dy \ .$$

To solve (1.3) for non-trivial M is hard and, as pointed out in the introduction, is also not necessary for our purposes. The relevant concept is instead that of a parametrix.

Def. 1.2: A parametrix of order N for L on M is function $K(x,y,t) \in C^\infty(MxMx]o,\infty[)$ such that

$$\begin{aligned} L_x K(x,y,t) &= O(t^{N/2-n/2}), \text{ uniformly in x on } MxMx]o,\infty[\\ B_x K(x,y,t) &= 0 \quad , \quad \partial MxMx]O,\ \infty[\\ K(x,y,0) &= \delta(x-y) \quad , \quad M \times M \times \{0\} \end{aligned} \tag{1.4}$$

The construction of parametrices will directly lead to AE of the kind indicated in the Introduction.

The first step in constructing K is the splitting ansatz,

$$K = K_0 - K_b$$

(K_0 = "free" part and K_b the boundary part). The problem (1.4) then

breaks up into two pieces:

$$
\begin{aligned}
&L_x K_0(x,y,t) = O(t^{N/t-n/\ell}) \\
(A)\quad &K_0(x,y,0) = \delta(x-y) \\
&L_x K_b(x,y,t) = O(t^{N/2-n/2}) \\
(B)\quad &B_x K_b(x,y,t) = B_x K_0(x,y,t) \quad , \ x\varepsilon\partial M \\
&K_b(x,y,0) = 0
\end{aligned}
$$

To solve (A) and (B) we shall employ the technique of reduction to the boundary (c.f. [Be], Chapter 3.7).

Before going into the details of this construction, let us fix some facts and notations concerning symbols and symbol classes, including some basic techniques from the theory of pseudodifferential operators (for a good reference, c.f. [Šub]).

The symbol of $P(x,D)$ will be $p(x,\xi) = \sum_{j=0}^{2} a_{2-j}(x,\xi)$ where $a_{2-j}(x,\xi)$ is homogenous in ξ of degree $(2-j)$. By ellipticity of P we have $a_2(a,\xi) \neq 0$ for $\xi \neq 0$. The symbol of L, $l(x,\xi,\tau)$ is then given by

$$l_2(x,\xi,\tau) = (i\tau + a_2(x,\xi))$$

$$l_{2-j}(x,\xi,\tau) = a_{2-j}(x,\xi) \quad , \quad j \neq 0$$

Note that $l_2(x,\xi,\tau)$ is homogenous of degree 2 in $(\xi,\tau^{1/2})$.

Def. 1.3: A function $a(x,\xi) \varepsilon C^\infty(MxR^n)$ is said to be a classical symbol of order m if one has the following asymptotic expansion

$$a(x,\xi) \sim \sum_{j=0}^{\infty} a_{m-j}(x,\xi) \quad , \tag{1.5}$$

where $a_{m-j}(x,\xi)$ is positively homogenous in ξ of degree $(m-j)$, i.e. $a_{m-j}(x,t\xi) = t^{m-j}a_{m-j}(x,\xi)$; $t>0$, $(x,\xi) \varepsilon Mx(R^n \setminus \{0\})$. We shall denote the set of classical symbols of order m by $S^m(Mx\ R^n)$ (or simply $S^m(M)$).

Remark 1.4: The notation $\sim$ in (1.5) signifies that for any $\ell>1$

$$a(x,\xi) - \sum_{j=0}^{\ell-1} a_{m-j}(x,\xi) \varepsilon S^{m-\ell}.$$

Given a classical symbol $a \in S^m(M \times R^n)$, we shall associate with it a classical pseudodifferential operator A of order m, by

$$Au(x) = \int e^{ix\cdot\xi} a(x,\xi)\hat{u}(\xi)d\xi \qquad (1.6)$$

($u \in$ the Schwartz space of rapidly decreasing functions). We shall denote by $L^m(M)$ the space of classical pseudodifferential operators of order m. For the properties of such operators we again refer to [Šub]. We shall be interested in inverting the operator L and to describe the inverse, we need to consider symbols depending on a parameter and we also need the basic results concerning composition of operators (again we refer to [Šub]). Let L^{-1} have symbol $q(x,\xi,\tau)$ for which we assume the asymptotic expansion

$$q(x,\xi,\tau) \sim \sum_{j=0}^{\infty} q_{-2-j}(x,\xi,\tau) \quad ,$$

with q_{-2-j} homogenous of degree $(-2-j)$ in $(\xi,\tau^{1/2})$ i.e.

$$q_{2-j}(x,t\xi,t^2\tau) = t^{-2-j} q_{-2-j}(x,\xi,\tau) \quad , \quad t>0 \quad .$$

The calculus of pseudodifferential operators now gives:

$$q_{-2}(x,\xi,\tau) = (i\tau + a_2(x,\xi))^{-1} \qquad (1.7)$$

$$q_{-2-p}(x,\xi,\tau) =$$

$$= -(i\tau+a_2(x,\xi))^{-1} \sum_{\substack{k+j+|\alpha|=p \\ j<p}} \partial_\xi^\alpha \, l_{2-k}(x,\xi,\tau) D_x^\alpha q_{-2-j}(x,\xi,\tau)/\alpha! \quad ,$$

for $p>0$.

In fact, for $p>0$, (1.7) can be compactly written as

$$q_{-2-p}(x,\xi,\tau) = \sum_{\ell=2}^{p+1} C_{\ell,p}(x,\xi)(i\tau+a_2(x,\xi))^{-\ell} \quad . \qquad (1.8)$$

$C_{\ell,p}(x,\xi)$ is here a polynomial in $p(x,\xi)$ and its derivatives up to a certain order depending on ℓ and p. We shall use (1.8) shortly in connection with higher order corrections

Solution of (A): Extend the problem to MxMx R by

$$K_0^+(x,y,t) = K_0(x,y,t)\chi(t>0)$$

($\chi(t>0)$ = characteristic function for the $t>0$ region). A simple calculation gives the jump formula:

$$LK_0^+(x,y,t) = (LK_0)^+(x,y,t) + K_0(x,y,0)\delta(t) = \delta(x-y)\delta(t)$$

(since we would like $(LK_0)^+ = 0$). So our problem is solved by

$$K_0^+(x,y,t) = L^{-1}\{\delta(x-y)\delta(t)\} = \int e^{i\langle x-y,\xi\rangle + it\tau} q(x,\xi,\tau)\,d\xi d\tau \qquad (1.9)$$

In view of the asymptotic expansion for $q(x,\xi,\tau)$ it is useful to define

$$K_{0N}^+(x,y,t) := \sum_{j=0}^{N} \int e^{i\langle x-y,\xi\rangle + it\tau} q_{-2-j}(x,\xi,\tau)\,d\xi d\tau := \sum_{j=0}^{\infty} \lambda_j^0(x,y,t).$$

From this one easily verifies

Lemma 1.5: With the above definition of $K_{0N}^+(x,y,\tau)$ and $\lambda_j^0(x,y,t)$, we have

1. $\lambda_j^0(x,x,t) = t^{\frac{-n-j}{2}} \lambda_j(x,x,1) := t^{\frac{-n-j}{2}} \alpha_j(x)$,
2. $\alpha_j(x) = 0$, for j odd
3. $K_{0N}^+(x,y,t)$ is a parametrix of order N (c.f. Def. 1.2),
4. $|K_0^+(x,y,t) - K_{0N}^+(x,y,t)| \le C\, t^{\frac{-n}{2} + \frac{N+1}{2}}$, uniformly in x.

Asymptotically, we therefore have

$$K_0^+(x,y,t) = K_{0N}^+(x,y,t) + O(t^{-n/2 + \frac{N+1}{2}}) \quad \text{for } t \text{ small and uniformly in } x.$$

Theorem 1.6: On the diagonal we have the asymptotic expansion

$$K_0(x,x,t) \underset{t\to 0+}{\sim} \sum_{\frac{j}{2} \in N_+} t^{-n/2+j/2} \alpha_j(x) \qquad (1.10)$$

Remark 1.7: We shall see that $\alpha_j(x)$ can be explicitly computed as polonomials in the symbol of L. The asymptotic expansion (1.10) can be integrated to yield

$$\Theta_p(t) = \mathrm{tr}(e^{-tp}) = \int_M K_0(x,x,t)\,dx \underset{t\to 0+}{\sim} \sum_{\frac{j}{2} \in N_+} t^{-n/2+j/2} \alpha_j \qquad (1.11)$$

with $\alpha_j := \int_M \alpha_j(x)dx$.

From the definition, $\alpha_j(x) := \lambda^0(x,x,1) =$

$$\int e^{i\tau} q_{-2-j}(x,\xi,\tau)d\xi d\tau = \sum_{\ell=2}^{j+1} \int e^{i\tau} c_{\ell,j}(x,\xi)(i\tau+a_2(x,\xi))^{-\ell} d\xi d\tau =$$

$$= \sum_{\ell=2}^{j+1} \int d\xi\ c_{\ell,j}(x,\xi)\ \frac{1}{(1-\ell)!}\ e^{-a_2(x,\xi)}, \quad j>0 .$$

In particular $\alpha_0(x) = \int d\xi\ e^{-a_2(x,\xi)}$, which can be easily computed to yield

$$\alpha_0(x) = \frac{1}{2}\Gamma(\tfrac{n}{2}) \int_{a_2(x,\xi)<1} d\xi , \text{ i.e. a kind of volume in } T^*(M).$$

In fact for a compact manifold without boundary (locally just an open subset of R^n), the volume is of course the basic geometric quantity to be measured. The other coefficients $\alpha_j(x)$, $j>0$ can be associated to more refined geometric quantities. However, before going into this, let us derive the analogue of (1.11) for problem (B).

Solution of (B): In a manner analogous to what we did when solving (A), we here extend the problem to $M\times M\times]0,\infty[$ by

$$K_b^+(x,y,t) = K_b(x,y,t)\chi(x_n>0)$$

which immediately gives the jump formula

$$LK_b^+(x,y,t) =$$

$$(LK_b(x,y,t)))^+ + g_0((x',0),y,t)\delta(x_n) + g_1((x',0),y,t)\delta'(x_n)$$

where (keeping the local normalization $a_{nj}(x',0) = 0$ for $j<n$ in mind):

$$g_0((x'0),y,t)) = -a_{nn}(x',0)\ \frac{\partial K_b}{\partial x_n}((x',0),y,t)+c_n(x',0)K_b((x',0),y,t)$$

$$g_1((x'0),y,t) = -a_{nn}(x',0)K_b((x',0),y,t) \qquad (1.12)$$

Now, $(LK_b)^+ = 0$ gives the formal solution

$$K_b^+(x,y,t) = L^{-1}\{g_0((x',0),y,t)\delta(x_n) + g_1((x',0),y,t)\delta'(x_n)\}. \qquad (1.13)$$

Additionally, we have the boundary conditions:

$$\lim_{x_n \to 0-} K_b^+(x,y,t) = 0$$

$$\lim_{x_n \to 0+} B_x K_b^+(x,y,t) = B_x K_0^+((x',0),y,t) \tag{1.14}$$

In fact, "forgetting" about the derivation of (1.12), we have the following reduction to the boundary result, which is basic for our approach

Theorem 1.8: Define $K_b^+(x,y,t) \in C^\infty(M\times M\times]0,\infty[)$ by (1.13). Under the conditions (1.14), g_0 and g_1 are then given as solutions to the pseudodifferential equations on ∂M:

$$g_0((x',0) = \Theta(x',D_x',D_t)g_1((x',0),y,t);$$

$$\Omega(x',D_x',D_t)g_1((x',0),y,t) = B_x K_0^+((x',0),y,t) \quad . \tag{1.15}$$

Here Θ and Ω are elliptic pseudodifferential operators of order 1, the explicit forms of which we shall give below.

Proof: A partial Fourier transform in (1.13) gives (forgetting about factors of (2π)):

$$K_b^+(x,y,t) =$$

$$\int e^{ix\cdot\xi+it\tau} q(x,\xi,\tau)\{\hat{g}_0((\xi',0),y,\tau) - i\xi_n \hat{g}_1((\xi',0),y,\tau)\}d\xi d\tau \tag{1.16}$$

with $q \sim \sum q_{-2-j}$.

Writing:

$$R_0 g_0 := \lim_{x_n \to 0-} \int e^{ix\cdot\xi+it\tau} q(x,\xi,\tau)\hat{g}_0((\xi',0),y,\tau)d\xi d\tau$$

$$R_1 g_1 := \lim_{x_n \to 0-} \int e^{ix\cdot\xi+it\tau} q(x,\xi,\tau) i\xi_n \hat{g}_1((\xi',0),y,\tau)d\xi d\tau$$

the first relation (1.14) amounts to $R_0 g_0 = R_1 g_1$. To render these expressions the form of psdo on ∂M, we need to carry out the ξ_n-integration and carry out the limit. To this end we write:

$$R_0(x',D_{x'},D_t)g_0((x',0),y,t): =$$
$$\int e^{ix'\cdot\xi'+it\tau}\rho^0(x',\xi',\tau)\hat{g}_0((\xi',0),y,\tau)d\xi'd\tau$$

$$R_1(x',D_{x'},D_x)g_1((x',0),y,t): =$$
$$\int e^{ix'\cdot\xi'+it\tau}\rho^1(x',\xi',\tau)\hat{g}_1((\xi',0),y,\tau)d\xi'd\tau$$

with

$$\rho^0(x',\xi',\tau):=\lim_{x_n\to 0-}\int e^{ix_n\xi_n}q(x,\xi,\tau)d\xi_n \sim \sum \rho^0_{-1-j}(x',\xi',\tau)$$

$$\rho^1(x',\xi',\tau):= \lim_{x_n\to 0-}\int e^{ix_n\xi_n}(i\xi_n)q(x,\xi,\tau)d\xi_n \sim \sum\rho^1_{-j}(x',\xi',\tau)\ .$$

Here, $\rho^0_{-1-j}(x',\xi',\tau): = \lim_{x_n\to 0-}\int e^{ix_n\xi_n}q_{-2-j}(x,\xi,\tau)d\xi_n$ and

$$\rho^1_{-j}(x',\xi',\tau): = \lim_{x_n\to 0-}\int e^{ix_n\xi_n}(i\xi_n)q_{-2-j}(x,\xi,\tau)d\xi_n \tag{1.17}$$

are homogenous in $(\xi',\tau^{1/2})$ of degree $(-1-j)$ and $(-j)$ respectively. This is seen as follows;

$$\rho^0_{-i-j}(x',t\xi',t^2\tau): = \lim_{x_n\to 0-}\int e^{ix_n\xi_n}q_{-2-j}(x,(t\xi',\xi_n),t^2\tau)d\xi_n=$$

$$= \lim_{x_n\to 0-}\int e^{ix_nt3_n}q_{-2-j}(x,t\xi,t^2\tau)td\xi_n =$$

$$= t^{-1-j}\lim_{x_n\to 0-}\int e^{ix_nt\xi_n}q_{-2-j}(x,\xi,\tau)d\xi_n$$

By a simple derivation argument or by actually computing the residue (using (1.8)), one sees that

$$\lim_{x_n\to 0-}\int e^{ix_nt\xi_n}q_{-2-j}(x,\xi,\tau)d\xi_n$$

is actually independent of t.
Consequently; $R_0\varepsilon\ L^{-1}(\partial M\times R)$, $R_1\ \varepsilon\ L^0(\partial M\times R)$ with symbols $\rho^0\varepsilon S^{-1}(\partial M\times R)$ and $\rho^1\ \varepsilon\ S^0(\partial M\times R)$.

To highest order we have:

$$\rho_{-1}^{0}(x',\xi',\tau) = \lim_{x_n \to 0-} \int e^{ix_n\xi_n}(i\tau+a_2(x,\xi))^{-1}d\xi_n$$

$$\rho_{0}^{1}(x',\xi',\tau) = \lim_{x \to 0-} \int e^{ix_n\xi_n}(i\xi_n)(i\tau+a_2(x,\xi))^{-1}d\xi_n \tag{1.18}$$

Now, as a function of ξ_n, $\xi_n \to (i\tau+a_2(x,\xi))$ has two simple zeroes, $\mu_{\pm}(x,\xi',\tau)$ in the $\overset{\text{upper}}{\text{lower}}$ half-planes. In fact $i\tau+a_2(x,\xi) = a_{nn}(x)(\xi_n-\mu_+)(\xi_n-\mu_-)$, where $\sum_{j\neq n} a_{jn}(x)\xi_j + \sum_{k\neq n} a_{nk}(x)\xi_k = -a_{nn}(x)(\mu_--\mu_+)$, so that on ∂M $(x_n = 0)$ we get

$$\mu_-((x',0),\xi',\tau) = -\mu_+((x',0),\xi',\tau) \tag{1.19}$$

(due to the normalization chosen, $a_{jn}(x',0) = 0$, $j\neq n$). Also, $\sum_{j,k\neq n} a_{jk}(x)\xi_j\xi_k + i\tau = a_{nn}(x)\mu_+\mu_-$ so that for $x_n=0$ we have

$$\mu_+((x',0),\xi'.\tau) = i\, a_{nn}(x',0)^{-1/2}\{\sum_{j,k\neq n} a_{jk}(x',0)\xi_j\xi_k+i\tau\}^{1/2} \tag{1.20}$$

Obviously $\mu_{\pm}((x',o),3',\tau)$ are elliptic symbols of order one,

$$\mu_{\pm}((x',0),t\xi',t^2\tau) = t\mu_{\pm}((x',0),\xi',\tau)$$

Similarly,

$$\frac{\partial a_2}{\partial \xi_n}((x',0),(\xi',\mu_{\pm}((x'0),\xi',\tau)) \equiv \frac{\partial a_2}{\partial 3_n}\Big/_{\substack{\xi_n=\mu_{\pm}\\ x_n=0}} =$$

$$= 2a_{nn}(x',0)\mu_{\pm}((x',0),\xi',\tau)$$

is also elliptic of order one. As for (1.18), a simple residue calculation now gives:

$$\rho_{-1}^{0}(x',\xi',\tau) = \lim_{x_n \to 0-} e^{ix_n\mu_-}\frac{1}{\frac{\partial a_2}{\partial \xi_n}(\xi_n=\mu_-)} = \frac{1}{2a_{nn}(x',0)\mu_-((x',0),\xi',\tau)}$$

$$\rho_0^1(x',\xi',\tau) = \lim_{x_n\to 0-} e^{ix_n\mu_-} \frac{i\mu_-}{\frac{\partial a_2}{\partial \xi_n}(\xi_n=\mu_-)} = \frac{i}{2\,a_{nn}(x',0)}$$

R_0, R_1 are hence elliptic and $R_0 g_0 = R_1 g_1$ yields immediately the first relation in (1.15) with

$$\theta(x',D_{x'},D_+) := R_0^{-1}R_1 \in L^1(\partial M\times R) \quad ,$$

which is obviously elliptic. Explicitly, assuming $R_0^{-1} \in L^1(\partial M\times R)$ has symbol $r(x',\xi',\tau)$ with expansion

$$r(x',\xi',\tau) \sim \sum r_{1-j}(x',\xi',\tau) \quad ,$$

$r_{1-j}(x',\xi',\tau)$ homogenous of order $1-j$ in $(\xi',\tau^{1/2})$, so that

$$r_1(x',\xi',\tau)=(\rho^0_{-1}(x',\xi',\tau)^{-1}=2a_{nn}(x',0)\mu_-((x',0),\xi',\tau) \ ,$$

$$r_{1-j}(x',\xi',\tau) =$$
$$=-(\rho^0_{-1}(x',\xi',\tau))^{-1} \sum_{k+\ell+|\alpha|=j} \partial^\alpha_{\xi'}\rho^0_{-1-k}(x',\xi',\tau)D^\alpha_{x'}r_{1-\ell}(x',\xi',\tau)/\alpha!$$

Then, denoting the symbol of θ by $\theta(x',\xi',\tau)$ we shall have an asymptotic expansion

$$\theta(x',\xi',\tau) \sim \sum \theta_{1-j}(x',\xi',\tau)$$

with

$$\theta_{1-j}(x',\xi',\tau) = \sum_{k+\ell+|\alpha|=j} \partial^\alpha_{\xi'}r_{1-k}(x',\xi',\tau)\ D^\alpha_{x'}\rho^1_{-\ell}(x',\xi',\tau)/\alpha!$$

In particular, for the principal symbol we obtain

$$\theta_1(x',\xi',\tau) = r_1(x',\xi',\tau)\rho_0^1 = i\mu_-((x',0),\xi',\tau)$$

The second relation in (1.15) is obtained by exploiting the second relation in (1.14). Let us consider

$$\lim_{x_n\to 0+} B_x K_b^+(x,y,t) = \lim_{x_n\to 0+} \sum_{k=1}^n b_k(x') \frac{\partial}{\partial x_k} K_b^+(x,y,t)$$

From (1.16) we obtain

$$\lim_{x_n\to 0+} \sum_{k=1}^{n} b_k(x') \int e^{ix\cdot\xi+it\tau} \{i\xi_k q(x,\xi,\tau)+\frac{\partial}{\partial x_k} q(x,\xi,\tau)\} *$$

$$(\hat{g}_0((\xi',0),y,t)-i\xi_n \hat{g}_1((\xi',0),y,\tau))d\xi d\tau = (\Delta_0+\Delta_{-1})g_0 + (H_1+H_0)g_1$$

Here, $\Delta_0, H_0 \in L^0(\partial M\times R)$, $\Delta_{-1} \in L^{-1}(\partial M\times R)$ and $H_1 \in L^1(\partial M\times R)$ have symbols $\delta^0 \sim \sum \delta^0_{-j}$, $\eta^0 \sim \sum \eta^0_{-j}$, $\delta^{-1} \sim \sum \delta^{-1}_{-1-j}$ and $\eta^1 \sim \sum \eta^1_{1-j}$ respectively. Explicitly:

$$\delta^0_{-j}(x',\xi',\tau) := \lim_{x_n\to 0+} \sum_{k=1}^{n} b_k(x') \int e^{ix_n\xi_n} i\xi_k q_{-2-j}(x,\xi,\tau)d\xi_n ,$$

$$\eta^0_{-j}(x',\xi',\tau) := \lim_{x_n\to 0+} \sum_{k=1}^{n} b_k(x') \int e^{ix_n\xi_n}(-i\xi_n)\frac{\partial}{\partial x_k} q_{-2-j}(x,\xi,\tau)d\xi_n ,$$

$$\delta^{-1}_{-1-j}(x',\xi',\tau) := \lim_{x_n\to 0+} \sum_{k=1}^{n} b_k(x') \int e^{ix_n\xi_n} \frac{\partial}{\partial x_k} q_{-2-j}(x,\xi,t)d\xi_n ,$$

$$\eta^1_{1-j}(x',\xi',\tau) := \lim_{x_n\to 0+} \sum_{k=1}^{n} b_k(x') \int e^{ix_n\xi_n}\xi_k\xi_n q_{-2-j}(x,\xi,\tau)d\xi_n .$$

(1.21)

Here δ^0_{-j}, η^1_{1-j}, η^0_{-j} and δ^{-1}_{-1-j} are homogenous of order -j, 1-j, -j and -1-j respectively. This is seen as follows;

$$\eta^1_{1-j}(x',t\xi',t^2\tau) =$$

$$= \lim_{x_n\to 0+} \sum_{k=1}^{n} b_k(x') \int e^{ix_n\xi_n}(t\xi_k)\xi_n q_{-2-j}(x,(t\xi',\xi_n),t^2\tau)d\xi_n =$$

$$= \lim_{x_n\to 0+} \sum_{k=1}^{n} b_k(x') \int e^{ix_n t\xi_n}(t\xi_k)(t\xi_n) q_{-2-j}(x,t\xi,t^2\tau)td\xi_n =$$

$$= t^{1-j} \lim_{x_n\to 0+} \sum_{k=1}^{n} b_k(x') \int e^{ix_n t\xi_n}\xi_k\xi_n q_{-2-j}(x,\xi,\tau)d\xi_n ,$$

and again one sees that

$$\lim_{x_n\to 0+} \sum_{k=1}^{n} b_k(x') \int e^{ix_n t\xi_n}\xi_k\xi_n q_{-2-j}(x,\xi,\tau)d\xi_n$$

does not depend on t. Analogously for the other symbols. Denoting

$\Delta_0+\Delta_{-1} = \Xi_0$ and $H_0+H_1 = \Xi_1$, we have

$$\lim_{x_n\to 0+} B_x K_b^+(x,y,t) = \Xi_0 g_0 + \Xi_1 g_1 \ , \quad \Xi_0 \varepsilon L^0(\partial M\times R),\ \Xi_1 \varepsilon L^1(\partial M\times R)$$

and both being elliptic. This is seen looking at the symbols

$$\zeta^0(x',\xi',\tau) = \delta^0(x',\xi',\tau)+\delta^{-1}(x',\xi',\tau);$$
$$\zeta^1(x',\xi',\tau) = \eta^0(x',\xi',\tau)+\eta^1(x',\xi',\tau) \ ,$$

which have principal parts;

$$\zeta_0^0(x',\xi',\tau) = \delta_0^0(x',\xi',\tau) =$$
$$= \frac{1}{2a_{nn}(x',0)} \Big(\sum_{k<n} b_k(x') i\xi_k \frac{1}{\mu_+((x',0),\xi',\tau)} + i\, b_n(x') \Big) \ ,$$
$$\zeta_1^1(x',\xi',\tau) = \eta_1^1(x',\xi',\tau) =$$
$$= \frac{1}{2\, a_{nn}(x',0)} \Big(\sum_{k<n} b_k(x')\xi_k + b_n(x')\mu_+((x',0),\xi',\tau) \Big) \ .$$

Using now the relation $g_0 = \Theta\, g_1$, we obtain:

$$\lim_{x_n\to 0+} B_k K_b^+(x,y,t) = (\Xi_0\, \Theta + \Xi_1) g_1 \ := $$
$$= Q(x',D_{x'},D_t) g_1((x',0),y,t) \ ,$$

which is the second relation (1.15).
Obviously; $Q(x',D_{x'},D_t) \varepsilon\ L^1(\partial M\times R)$ and for the symbol we have the expansion

$$\omega^1 \sim \sum \omega^1_{1-j}$$

where,

$$\omega^1_{1-j}(x',\xi',\tau) =$$
$$= \sum_{k+\ell+|\alpha|=j} \partial_\xi^\alpha \cdot \zeta^0_{-k}(x',\xi',\tau) D_{x'}^\alpha \cdot \Theta_{1-\ell}(x',\xi',\tau)/\alpha! + \zeta^1_{1-j}$$

and principal symbol

$$\omega_1(x',\xi',\tau) = \zeta_0^0\theta_1 + \zeta_1^1 =$$

$$= \frac{1}{a_{nn}(x',0)} \left(\sum_{k<n} b_k(x')\xi_k + b_n(x')\mu_+((x',0),\xi',\tau) \right) .$$

This ends the proof of Theorem 1.8.

The formalism which has been set up for the proof will now easily yield the asymptotic expansion for $K_b^+(x,x,t)$. Our next step is therefore to prove the analogue of Lemma 1.5. The calculus above will also yield the explicit form of geometric quantities.

2. The Asymptotic Expansion for $K_b^+(x,x,t)$

This section aimes at proving results for $K_b^+(x,y,t)$ analogous to Lemma 1.5. As a result we then also abtain the asymptotic expansion for the total parametrix $K = K_0 - K_b$.

The starting point will be Theorem 1.8. Solving for g_1 in

$$\Omega(x',D_{x'},D_t)g_1((x',0),y,t) = \lim_{x_n \to 0+} B_x K_0^+(x,y,t) \qquad (*)$$

and computing g_0 from

$$g_0((x',0),y,t) = \theta(x',D_{x'},D_t)g_1((x',0),y,t) , \qquad (**)$$

we have all the information necessary to expand $K_b^+(x,x,t)$. We are first only interested in homogeneity properties of $\hat{g}_0((\xi',0),y,t)$ and $\hat{g}_1((\xi',0),y,\tau)$ in $(\xi',\tau^{1/2})$ and such properties are almost automatic from the calculus built up in the previous section.

From (1.9), $K_0^+(x,y,t) = L^{-1}(x,D_x,D_t)\delta(x-y)\delta(t)$ and we denote $f_y(x,t) = \delta(x-y)\delta(t)$ so that $\hat{f}_y(\xi,\tau) = e^{-iy\xi}$. Let $\Sigma := B_x \cdot L^{-1}$ with symbol $\sigma(x,\xi,\tau) = \beta(x',\xi) \cdot q(x,\xi,\tau)$ (symbol product) where $\beta(x',\xi)$ = symbol $B_x = \sum_{k=1}^{n} b_k(x')i\xi_k$. Then

$$\lim_{x_n \to 0+} B_x K_0^+(x,y,t) = \lim_{x_n \to 0+} \Sigma(x,D_x,D_t)f_y(x,t) =$$

$$= \int e^{ix'\cdot\xi' + it\tau} \left(\lim_{x_n \to 0+} \int e^{ix_n\xi_n} \sigma(x,\xi,\tau) e^{-iy_n\xi_n} d\xi_n \right) \hat{f}_{y'}(\xi',\tau) d\xi' dt.$$

Let $\phi(x',\xi',\tau;y_n) = \lim_{x_n \to 0+} \int e^{ix_n\xi_n} \sigma(x,\xi,\tau) e^{-iy_n\xi_n} d\xi_n$ (parameter y_n),

and denote the corresponding operator by $\Phi(x',D_{x'},D_t)$. Note that $\phi(x',t\xi',t^2\tau;t^{-1}y_n) = \phi(x',\xi',\tau;y_n)$, σ being of order -1. Using (*) and inverting Ω we find that

$$\hat{g}_1((\xi',0),y,\tau) = (\text{elliptic factor of order } -1)\cdot e^{-iy\xi}$$

and from (**)

$$\hat{g}_0((\xi',0),y,\tau) = (\text{elliptic factor of order } 0)\cdot e^{-iy\xi}.$$

Lemma 2.1: $K_b^+(x,x,t)$ has an asymptotic expansion

$$K_b^+(x,x,t) \underset{t\to 0+}{\sim} \sum_{j\in N_+} \lambda_j^b(x,x,1)t^{\frac{-n-j}{2}} \tag{2.1}$$

Proof: Writing

$$K_b^+(x,y,t) =$$

$$\sum_j \int e^{ix\cdot\xi+it\tau} q_{-2-j}(x,\xi,\tau)\{\hat{g}_0((\xi',0),y,\tau)-i\xi_n\hat{g}_1((\xi',0),y,\tau)\}d\xi d\tau$$

$:= \sum \lambda_j^b(x,y,t)$ we find that $\lambda_j^b(x,x,t) = t^{\frac{-n-j}{2}}\lambda_j^b(x,x,1)$ by the usual change of argument combined with homogeneity properties of $\hat{g}_0,\hat{g}_1$. We also find the analogous properties to those stated in Lemma 1.5, which gives the asymptotic expansion (2.1).

We therefore have the asymptotic expansion for $K=K_0-K_b$;

$$K(x,x,t) \underset{t\to 0+}{\sim} t^{-n/2}\left\{\sum_{j/2\in N_+} t^{+j/2}\alpha_j(x) + \sum_{j\in N_+} t^{j/2}\lambda_j^b(x,x,1)\right\} \tag{2.2}$$

Furthermore, the calculus above yields computable expressions for the expansion coefficients $\alpha_j(x)$, $\lambda_j(x,x,1)$ to any order. These coefficients we shall identify with geometric quantities later. Note, that unlike the free case, $\lambda_j^b(x,x,1)$ do not vanish in general for odd j.

3. Global Results

The construction has so far been purely local (c.f. (1.2)). It is however a routine matter to show that the local results obtained

so far can be patched together to yield a global construction. For this, let $\{U_\nu\}$ be a (finite) covering of M and Ψ_ν a subordinated partition of unity. Define (writing K just for either K_0 or K_b)

$$K_{N,\nu}(x,y,t) := \Psi_\nu(x)K_N(x,y,t)\Psi_\nu(y)$$

(where K_N are just the sum of the N first terms in the expansion of K) and globally

$$K_N(x,y,t) = \sum_\nu K_{j,\nu}(x,y,t) \quad .$$

The construction above then yields (2.2) uniformly on M.

4. Microlocalized Spectral Geometry for Closed Manifolds.

As indicated in the Introduction, we shall in this section be concerned with a reduction process. By this process we shall break down the geometric information in asymptotic expansions for general P(x,D) to that associated with the 1-parameter semigroup of translations.

The tools for the reduction process will be a combination of microlocal analysis and a simple semigroup argument.

As for microlocal analysis in general, we refer to [Tr]. The essential idea is here that many objects in the usual theory of pseudodifferential operators can be naturally localized in the cotangent bundle $T^*(M)$, not just in M. Locally in $T^*(M)$ (microlocally) a considerable simplification in the structure of these objects can sometimes be achieved. A general PDO, say P(x,D) can, e.g., depending on the algebraic geometry of its characteristic set, be microlocally reduced at a generic point in $T_0^*(M)$ to operators like

$$D_1, \; D_1 + i\,D_2 \quad \text{and} \quad D_1 + ix_1D_2 \, , \quad (D_j \equiv i\frac{\partial}{\partial x_j})$$

(c.f. the more standard reduction of a non-degenerate vector field X to the form D_1 locally).

As usual, the global situation is controlled by inverting the transformations used and by patching together the local solutions by means of a partition of unity.

For the sake of brevity we shall here only sketch the arguments and only in the case of a closed manifold (c.f. the Introduction for

$\partial M \neq \emptyset$).

Let in this section $P(x,D)$ be an m:th order elliptic PDO with homogeneous (of order m) positive principal symbol $p_m(x,\xi)$.

Theorem 4.1: The asymptotics $\theta_P(t) \underset{t\to 0+}{\sim}$ is determined by the asymptotics for $\theta_{D_n}(t)$.

Proof: This reduction is done in steps. Let $Q: \equiv P^{1/m}$, then Q is a first order psdo (pseudodifferential) with principal symbol $p_m(x,\xi)^{1/m}$. For elliptic first order psdo an asymptotic expansion can be derived essentially as in the PDO case (c.f. [Du-Guil]). By the comment in the Introduction the asymptotic expansion for $\theta_Q(t)$ determines that for $\theta_P(t)$. Hence we may study only $\theta_Q(t)$. Microlocally at a generic point $(x_0,\xi_0) \in T_0^*(M)$ one can find an elliptic (in a conic neighbourhood of (x_0,ξ_0)) Fourier integral operator F (of any order) such that $F\,QF^{-1}$ and D_n are microlocally conjugate (at (x_0,ξ_0)) to each other (c.f. [Tr] p. 471). This means that

$$(x_0,\xi_0) \notin \mu \text{ supp } (FQF^{-1}-D_n)$$

(where μ supp (A) denotes the microsupport of A). So there exists a regularizing operator $B \in L^{-\infty}(M)$ such that near (x_0,ξ_0), we have $FQF^{-1} - D_n = B$. Now, $\theta_Q(t) = \mathrm{tr}(e^{-tQ}) = \mathrm{tr}(Fe^{-tQ}F^{-1}) = \mathrm{tr}(e^{-tFQF^{-1}})$ and near (x_0,ξ_0) this equals

$$\mathrm{tr}(e^{-t(D_n+B)}) \quad .$$

Clearly $\lim_{t\to 0+} \| e^{-t(D_n+B)} - e^{-tD_n} \| = 0$ since $B \in L^{-\infty}$. This follows from $e^{-tB} - e^{-t(D_n+B)} = \int_0^t e^{-(t-s)D_n} B\, e^{-s(D_n+B)}\, ds$ and by the same argument convergence in the trace-norm also follows, i.e.,

$$\mathrm{tr}(e^{-t(D_n+B)}) = \mathrm{tr}(e^{-tD_n}) \text{ , for small } t.$$

Hence, microlocally at a generic point we have for small t

$$\theta_Q(t) = \theta_{D_n}(t) \quad .$$

Remark 4.2: $\frac{\partial}{\partial x_n}$ is of course the generator of translation in the x_n-direction (with domain $D = H^{1,p}$ (in the x_n-direction)), i.e.,

$e^{-tD_n} f(x_n) = f(x_n + it)$. e^{-tD_n} has thus the integral kernel $K(x_n, y_n; t) = \delta(x_n - y_n + it)$.

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