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ASYMPTOTIC EXPANSION OF THE HEAT KERNEL FOR A CLASS OF HYPOELLIPTIC OPERATORS

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Introduction. Let M be a smooth compact manifold without boundary, let dx be a fixed positive smooth density on M, and let $X_1, \ldots, X_l$ be smooth real vector fields on M, i.e. in a local coordinate system, $X_j = \sum_{i=1}^n a_j^i \partial_{x_i}$. We will consider operators A of the form (m is even)

$$(1)\qquad (-1)^{m/2} \sum_{j=1}^{l} X_j^m + \sum_{|\alpha|<m} a_\alpha(x) X^\alpha$$

where $\alpha = (\alpha_1, \ldots, \alpha_k)$, $X^\alpha = X_{\alpha_1} \ldots X_{\alpha_k}$, $|\alpha| = k$ and the a_α are smooth functions. The well-known example is the sum of the squares of vector fields,

$$(2)\qquad -\sum_{j=1}^{l} X_j^2 + X_0 + c(x)\,.$$

A result of Hörmander [7, 14] states that this operator is hypoelliptic if the vector fields $X_1, \ldots, X_l$ and all their commutators $[X_{i_1}, [X_{i_2} \ldots [X_{i_{s-1}}, X_{i_s}] \ldots], s \le r$, up to length r span the tangent space to M at each point. We recall that an operator A is said to be *hypoelliptic* on M if for any open set $U \subset M$ and distributions u, f on U satisfying $Au = f$, $f \in C^\infty(U)$ implies $u \in C^\infty(U)$. In [17] for the operator (2) it was shown (with $m = 2$) that

$$\|u\|_{m/r} \le C(\|Au\|_0 + \|u\|_0)\,,$$

for all $u \in C^\infty(M)$, where $\|\cdot\|_s$ denotes the norm in the usual Sobolev space $H_s(M)$. For the operator (1) this estimate and hypoellipticity were proved in [6, 16].

We assume that the operator (1) is formally selfadjoint and positive, that is, $(Au, v) = (u, Av)$ and $(Au, u) \ge 0$ for all $u, v \in C^\infty(M)$. It is easy to show that under our assumption A is an unbounded selfadjoint operator on the domain $D_A = \{u \in H_{m/r}(M) : Au \in L_2(M)\}$ and has discrete spectrum $\lambda_j \to \infty$. Let $U(x, y, t)$ be the kernel of the operator $\exp(-tA)$,

$$U(x, y, t) = \sum_{j=1}^{\infty} e^{-\lambda_j t} \varphi_j(x) \varphi_j(y) .$$

Here $\varphi_j(x)$ is a complete orthonormal set of eigenfunctions of A with eigenvalues $\{\lambda_j\}$. $U(x, y, t)$ is a fundamental solution for the operator $L = \partial_t + A$ and so it is called the *heat kernel* for L.

We denote by $V_k(x)$ the subspace of $T_x(M)$ spanned by $X_1, \ldots, X_l$ and all their commutators of length $\le k$ and let $\nu_k(x) = \dim V_k(x)$ $(\nu_0 = 0)$. We say that *Hörmander's condition* (of order r) *holds* if

$$\nu_r(x) = \dim M = n \quad \text{for all } x \in M .$$

We will also use the condition introduced by Métivier [13]:

$$\nu_k(x) = \nu_k = \text{const} , \quad 1 \le k \le r, \text{ for all } x \in M .$$

Our main results are the following.

THEOREM 1. *If Hörmander's condition holds then the heat kernel for the operator* (1) *has the following asymptotic expansion as* $t \to +0$:

$$U(x, x, t) = \sum_{j=-q(x)}^{\infty} c_j(x) t^{j/m} + \sum_{j=0}^{\infty} d_j(x) t^{j/m} \ln(t) \tag{3}$$

where $q(x) = \sum_{k=1}^{r} (\nu_k(x) - \nu_{k-1}(x)) k$, *and* $c_j(x)$, $d_j(x)$ *are some functions on* M.

We remark that in general this expansion is not uniform in $x \in M$ and the functions c_j, d_j are not continuous.

THEOREM 2. *In the Métivier case the asymptotics in Theorem* 1 *is uniform in* $x \in M$, $c_j(x), d_j(x) \in C^\infty(M)$, *and as* $t \to +0$,

$$\operatorname{tr} \exp(-tA) = \sum_{j=-q}^{\infty} c_j t^{j/m} + \sum_{j=0}^{\infty} d_j t^{j/m} \ln(t) \tag{4}$$

where $q = \sum_{k=1}^{r} (\nu_k - \nu_{k-1}) k$.

It is also possible to find the leading coefficient $c_{-q(x)}(x)$ explicitly (see below). For elliptic operators this result is well known; in this case $q = \dim M$ and in addition all $d_j = 0$. For the operator (2) our results were obtained independently by G. Ben Arous [2, 3], who used probabilistic methods. Formula (4) was also proved in [19] for $r = 2$, and related results were obtained in [1, 18]. D. Jerison and A. Sánchez-Calle [8, 9, 15] estimated the kernel $U(x, y, t)$ in terms of the metric associated with the operator A. From the asymptotics of the heat kernel it is easy to find the first term of the asymptotics of the spectral function of A [10–12] (for second order operators in the Métivier case this was done by a different method by G. Métivier [13]). To prove Theorems 1, 2 we use the method developed in [3, 7, 8].

1. Dilations and homogeneity. In this section we recall some definitions and propositions connected with homogeneous structures (see [4, 5, 15, 17] for details). Let $e_1, \ldots, e_n$ be a basis in $\mathbb{R}^n$ and let $0 = \nu_0 < \nu_1 < \ldots < \nu_r$ be integers. We write $[j] = k$ if $\nu_{k-1} < j \le \nu_k$. We define a group of linear automorphisms δ_s of $\mathbb{R}^n$ by

$$\delta_s(e_j) = s^{[j]} e_j\,, \qquad 1 \le j \le n\,.$$

We also consider a homogeneous norm $\|\cdot\|$ with respect to δ_s such that

$$\|u\| = 0 \;\Leftrightarrow\; u = 0, \qquad \|\delta_s(u)\| = s\|u\|\,.$$

For example we can take $\|u\| = (\sum_{j=1}^n |u_j|^{2/[j]})^{1/2}$. This norm satisfies the following inequalities:

$$\|u+v\| \le C(\|u\| + \|v\|), \qquad C_1|u| \le \|u\| \le C_2|u| \quad \text{for } |u| \le C\,,$$

where $|\cdot|$ is the usual euclidean norm in $\mathbb{R}^n$. The number $q = \sum_{k=1}^r (\nu_k - \nu_{k-1})k$ is called the *homogeneous dimension* of the space. It is easy to see that $\mathbb{R}^n = \bigoplus_{k=1}^r V_k$, V_k is spanned by the vectors e_j for $[j] = k$, and $q = \sum_{k=1}^r k \dim V_k$.

A function f is *homogeneous* of degree λ if $f \circ \delta_s = s^\lambda f$ for all $s > 0$. A distribution v is *homogeneous* of degree λ if $\langle v, \varphi \circ \delta_s\rangle = s^{Q-\lambda}\langle v, \varphi\rangle$. A function $k(u)$ is said to be a *kernel of type* λ if it is smooth away from the origin and homogeneous of degree $-Q + \lambda$. A differential operator T is *homogeneous* of degree λ if $T(f \circ \delta_s) = s^\lambda (Tf) \circ \delta_s$ for all $s > 0$. For example, the function $u^\alpha = u_1^{\alpha_1} \ldots u_n^{\alpha_n}$ is homogeneous of degree $[\alpha] = \sum_{j=1}^n \alpha_j [j]$, the operator $u^\alpha \partial/\partial u_j$ is homogeneous of degree $[j] - [\alpha]$. Let U be a neighborhood of the origin in $\mathbb{R}^n$. We define the function space

$$C_m^\infty(U) = \{f(u) \in C^\infty(U) : |f(u)| = O(\|u\|^m),\ u \to 0\}\,.$$

A differential operator $T = \sum_{|\alpha| \le k} a_\alpha(u)\partial_u^\alpha$ from $C^\infty(U)$ to $C^\infty(U)$ is said to have *degree at most* p at 0 whenever $T(C_m^\infty(U)) \subset C_{m-p}^\infty(U)$ for all $m \in \mathbb{N}$. For such an operator it is possible to define an operator $\widehat{T}$,

$$\widehat{T} = \sum_{|\alpha| \le k} \; \sum_{[\beta] \le [\alpha] - p} (\partial_u^\beta a_\alpha(0) u^\beta / \beta!)\partial_u^\alpha\,,$$

which is homogeneous of degree p. The operator $T - \widehat{T}$ has degree at most $p - 1$ at 0.

Let $\mathfrak{g}$ be a free nilpotent Lie algebra of step r with l generators, $\mathfrak{g} = \bigoplus_{k=1}^r \mathfrak{g}_k$, and $[\mathfrak{g}_i, \mathfrak{g}_j] = \mathfrak{g}_{i+j}$ if $i + j \le r$, $[\mathfrak{g}_i, \mathfrak{g}_j] = 0$ if $i + j > r$. Using the exponential mapping we can identify $\mathfrak{g}$ and the corresponding Lie group G; the group multiplication in $\mathfrak{g}$ will be given by the Campbell–Hausdorff formula

$$u \cdot v = u + v + [u, v] + \ldots, \qquad u, v \in \mathfrak{g}\,.$$

Following [15] we now define a function class F_λ : $k \in F_\lambda$ if

(i) $k \in C^\infty(\mathfrak{g} \setminus 0), k(u) = 0$ for $\|u\| > 1$,

(ii) $|Pk(u)| \le C_s(1+\|u\|^{\lambda-Q-s})$, for all left-invariant differential operators P homogeneous of degree s.

We will also use another class HF_λ. A function k is in HF_λ if $k \in F_\lambda$ and

(i) if $\lambda < Q$ then $k(u) = \widehat{k}(u) + g(u)$, where $\widehat{k}(u)$ is a kernel of type $\lambda, g(u) \in C^\infty(\mathfrak{g})$,

(ii) if $\lambda \ge Q$ then (i) holds for the function Pk for all left-invariant differential operators P of degree s, $\lambda - s < Q$.

LEMMA 1. 1) *If k is a kernel of type $\lambda, \varphi \in C_0^\infty(\mathfrak{g})$ and $\varphi(u) = 1$ for $\|u\| \le 1/2$, then $\varphi k \in HF_\lambda$ and $P\varphi k \in HF_{\lambda-s}$ for P homogeneous of degree s.*

2) *If $k \in HF_\alpha$, h is a kernel of type $\beta, 0 < \beta < Q, \alpha > 0$ and $\varphi \in C_0^\infty(\mathfrak{g})$ with $\varphi(u) = 1$ for $\|u\| \le 1/2$ then $\varphi(k * h) \in HF_{\alpha+\beta}$.*

P r o o f. We have $\varphi k = \widehat{k} + g$ with $\widehat{k} = k$ and $g = (1-\varphi)k(u) \in C^\infty(\mathfrak{g})$ since $k(u)$ is a kernel of type λ, so $\varphi k \in HF_\lambda$. For $P\varphi k$ we observe that since $\varphi = 1$ in a neighborhood of the origin, $P\varphi k - \varphi Pk \in C_0^\infty$; since Pk is a kernel of type $\lambda - s$, we have $P\varphi k \in HF_\lambda$ and 1) is proved.

For 2) we observe that if $\alpha + \beta < Q$ then by definition $k(u) = \widehat{k}(u) + g(u)$, so $k*h(u) = \int k(v)h(v^{-1}u)\,dv = \int \widehat{k}(v)h(v^{-1}u)\,dv + \int g(v)h(v^{-1}u)\,dv = I_1 + I_2$. I_1 is a kernel of type $\alpha+\beta$ by the result of Folland [4], $I_2(u)$ is a smooth function, and using the same arguments as in Lemma 3 of [15] one can see that $g = I_2$ satisfies the required estimate. In the case $\alpha+\beta \ge Q$ we have $P(k*h) = (Pk)*h$, Pk is a kernel of type $\lambda - s$, and $\lambda - s + \beta < Q$, so as was shown before $\varphi P(k*h) \in HF_{\alpha+\beta-s}$ and by definition $k * h \in HF_{\alpha+\beta}$.

We say that a function k is in SF_λ if for any $s \in \mathbb{N}$ with $s > \lambda$,

$$k(u) = \sum_{j=0}^{s} k_j(u) + q_s(u)\,,$$

where $k_j \in HF_{\lambda+j}$ and $q_s \in F_s(\mathfrak{g})$.

2. Lifting of vector fields. Let $L(M)$ be the Lie algebra of smooth real vector fields on M. There exists a partial homomorphism $\mu : \mathfrak{g} \to L(M)$, that is, μ is linear and for all $a \in \mathfrak{g}_i$, $b \in \mathfrak{g}_j$ we have $\mu([a,b]) = [\mu(a), \mu(b)]$ if $i + j \le r$. Write $\mu_x(a) = \mu(a)|_x$, $x \in M$.

We now define

$$H_k(x) = \{a \in \mathfrak{g}_k : \mu_x(a) \in V_{k-1}(x)\}, \qquad 1 \le k \le r\,, \qquad H(x) = \bigoplus_{k=1}^{r} H_k(x)\,.$$

We select $S_k(x)$ such that $\mathfrak{g}_k = H_k(x) \oplus S_k(x)$, and set $S(x) = \bigoplus_{k=1}^{r} S_k(x)$. As was shown in [5], $H(x)$ is a subalgebra in $\mathfrak{g}$, $\dim S_k(x) = \nu_k(x) - \nu_{k-1}(x)$ and

$\dim S(x) = \dim M$. Obviously $q(x)$ is the homogeneous dimension of $S(x)$, and $q(x) + \beta(x) = Q$, where $\beta(x)$ is the homogeneous dimension of $H(x)$.

We now change the local coordinate system in a neighborhood of $x \in M$ so that in the new coordinates the vector fields $X_1, \ldots, X_l$ have degree at most one. It is easy to see that $S(x) = \mathfrak{g}/H(x)$; let γ be a projection from $\mathfrak{g}$ to $S(x)$. The essential result in this situation is

THEOREM 3 (Helffer–Nourrigat [5]). *For any $x \in M$ there exists a diffeomorphism $\Theta_x : U \to \omega$, where U is a neighborhood of* 0 *in $S(x)$ and ω is a neighborhood of x in M, so that if $\mu(a) = X$ then*

1) $(\widehat{\Theta_x^{-1}})_* X = \widehat{X}, \quad \widehat{X} f(u) = \dfrac{d}{dt}\Big|_{t=0} f(\gamma(u \cdot ta))$;
2) $(\Theta_x(0))_*(0) = \mu_x|_{S(x)}$.

In the Métivier case Θ_x is smooth in $x \in M$.

We introduce coordinates (u, v) in $\mathfrak{g}$ so that $u \in S(x)$, $v \in H(x)$. If $\mu(a) = X_i$ $(1 \le i \le l)$ we define a left-invariant vector field Y_i on $\mathfrak{g}$ by $Y_i f(u, v) = (d/dt)|_{t=0} f((u, v) \cdot ta)$. Consequently,

$$Y_i(f \cdot \gamma) = \frac{d}{dt}\Big|_{t=0} f(\gamma((u, v)) \circ ta) = (\widehat{X}_i f) \circ \gamma\,.$$

Let $R_i = X_i - \widehat{X}_i$, $1 \le i \le l$. By Theorem 3 the vector fields R_i have degree at most 0 at 0. If we now define $\widetilde{X}_i = Y_i + R_i$ then we obtain

LEMMA 2. *$\widetilde{X}_i(f \circ \gamma) = (X_i f) \circ \gamma$ for $1 \le i \le l$.*

3. Construction of the fundamental solution. We will consider two differential operators connected with L:

$$\widetilde{L} = (-1)^{m/2} \sum_{j=1}^{l} \widetilde{X}_j^m + \sum_{|\alpha| < m} a_\alpha(x) \widetilde{X}^\alpha + \frac{\partial}{\partial t}\,, \qquad \widehat{L} = (-1)^{m/2} \sum_{j=1}^{l} Y_j^m + \frac{\partial}{\partial t}\,.$$

LEMMA 3. *The operator $\widehat{L}$ is hypoelliptic.*

Proof. For $m = 2$ this follows directly from Hörmander's theorem. In the case $m > 2$ it can be shown by using a criterion of hypoellipticity by Helffer–Nourrigat [6] (see also [12]).

On $\mathfrak{g}' = \mathfrak{g} \times \mathbb{R}^1$ we define dilations by $\delta_s(\xi, t) = (\delta_s(\xi), s^m t)$, $\xi \in \mathfrak{g}'$, $t \in \mathbb{R}^1$. Then $Q' = Q + m$ is the homogeneous dimension of $\mathfrak{g}'$. For $\mathfrak{g}'$ we can define the spaces F_λ, HF_λ, SF_λ as in the previous section. It is clear that Lemma 1 is true in this situation. The operator $\widehat{L}$ is homogeneous on $\mathfrak{g}'$ of degree m. By a result of G. B. Folland [4] we can find a kernel $k(\xi, t)$ of type m which is a fundamental solution for $\widehat{L}$, that is,

$$\widehat{L}k = \delta(\xi, t) \tag{5}$$

in the sense of distributions, where δ is the delta distribution on $\mathfrak{g}'$.

We denote by U, U_1 neighborhoods of the origin in $S(x)$, and by V, V_1 neighborhoods of the origin in $H(x)$ which are sufficiently small and satisfy $U \Subset U_1$, $V \Subset V_1$. Let $\varphi \in C_0^\infty(U_1)$, $\varphi = 1$ on U, $\psi \in C_0^\infty(V_1)$, $\psi = 1$ on V, and $\varrho(t) \in C_0^\infty(-2, 2)$, $\varrho(t) = 1$ for $|t| < 1$. We now define

$$k_0(\xi, t) = \varphi\psi\varrho k(\xi, t)\,.$$

From the definitions of the operators $\widehat{L}$ and $\widetilde{L}$ we see that

$$\widetilde{L} = \widehat{L} + R\,,$$

where R has degree at most $m - 1$. Consequently, for any $s \in \mathbb{N}$, the operator $\widetilde{L}$ can be written in the form

$$\widetilde{L} = \widehat{L} + \sum_{i=1}^{s} R_i + Q_s\,,$$

where the R_i are homogeneous operators of degree $m - i$ and Q_s has degree at most $m - s - 1$ at 0. Using (5) and Lemma 1 we obtain

$$\widetilde{L}k_0(\xi, t) = \varphi\psi\varrho \cdot \delta + \sum_{i=1}^{s} \varphi\psi\varrho k r_i + q_s \tag{6}$$

for $\xi \in U_1 \times V_1, t \in (-2, 2)$, where $r_i \in HF_i$, $q_s \in F_{s+1}$.

LEMMA 4. *Given $s \in \mathbb{N}$ there exists a function $K_s(\xi, t) \in SF_m$ such that*

$$\widetilde{L}K_s = \varphi\psi\varrho \cdot \delta + H_s, \qquad H_s \in SF_s\,.$$

P r o o f. We use induction on s. For $s = 0$ we set $K_0(\xi, t) = k_0(\xi, t)$, and the statement of the lemma follows from (6). Assume that it is true for $s - 1$; then we have

$$\widetilde{L}K_{s-1} = \varphi\psi\varrho \cdot \delta + H_{s-1}, \qquad H_{s-1} \in SF_{s-1}\,.$$

We now define $K_s(\xi, t)$ by $K_s = K_{s-1} - a(\xi, t)k_0 * H_{s-1}$, where $a(\xi, t) \in C_0^\infty(\mathfrak{g}')$, $\operatorname{supp} a \subset U_1 \times V_1 \times (-2, 2)$ and $a \equiv 1$ in $\operatorname{supp} H_{s-1}$. We have

$$\widetilde{L}K_s = \varphi\psi\varrho \cdot \delta + H_{s-1} - aH_{s-1} + H_s\,,$$

where $H_s = a(\xi, t)\widehat{L}k_0 * H_{s-1} - \widetilde{L}(a(\xi, t)k_0 * H_{s-1})$. By Lemma 1 it is clear that $K_s(\xi, t) \in SF_m$, $H_s \in SF_s$ and the proof is finished.

By Sobolev's embedding theorem for any $p \in \mathbb{N}$ there exists s so that $SF_\lambda \subset C^p(\mathfrak{g})$. From this fact and the previous lemma

$$\widetilde{L}K_s = \varphi\psi\varrho \cdot \delta + H_s, \qquad H_s \in C^s(\mathfrak{g})\,.$$

We now want to construct a fundamental solution for the original operator L. Set

$$p_s(u, t) = \int K_s(u, v, t)\,dv, \qquad h_s(u, t) = \int H_s(u, v, t)\,dv\,.$$

LEMMA 5. $Lp_s = \varphi\varrho \cdot \delta + h_s$.

Proof. Let $R = L - \widetilde{L}$. Then

$$Lp_s = \varphi\varrho \cdot \delta + h_s - \int RK_s\,dv + \int RH_s\,dv\,.$$

The operator R is selfadjoint and acts only in the v variables so it is easy to see that $\int RK_s\,dv = 0$ and $\int RH_s\,dv = 0$, and the lemma is proved.

Using the second property of the map Θ from Theorem 3 one can show that in the original coordinate system (y) in some small neighborhood ω of the point $x \in M$,

$$Lv(x)p_s = \delta + h_s\,,$$

where $v(x) = |\det(\mu_x|_{S(x)})|$. This formula and Lemma 5 imply that

$$U(x,x,t) = v(x)p_s(0,t) + g(t)\,, \tag{7}$$

where $g(t) \in C^s(\omega \times (-1,1))$. By construction,

$$p_s(0,t) = \sum_{j=1}^{s} \int k_j(0,v,t)\,dv + \ldots$$

If $k_j \in HF_\lambda$ for $\lambda < \beta(x)$ then by definition of this class

$$\int k_j(0,v,t)\,dv = \int \widehat{k}_j(0,v,t)\,dv + \int g_j(0,v,t)\,dv\,.$$

Consequently, $p_j(0,t) = \widehat{p}_s(0,t) + g(t)$, where $\widehat{p}_s(0,t)$ is homogeneous of degree $\lambda - \beta(x)$ and $g \in C^\infty(-1,1)$.

If $\lambda > \beta(x)$ then we have

$$\partial_t^a p_j(0,t) = \int \partial_t^a k_j(0,v,t)\,dv + \int \partial_t^a c(0,v,t)\,dv = \widehat{p}_j(0,t) + g(t)\,.$$

The function $\widehat{p}_j(0,t)$ is homogeneous of degree $(j-Q)/m-a$. If $(j-Q)/m-a \notin \mathbb{Z}$ then $\widehat{p}_j = c_j t^{(j-Q)/m-a}$, and after integrating over t we obtain

$$p_j(0,t) = c_j t^{(j-Q)/m} + g(t)\,, \tag{8}$$

$g \in C^\infty(-1,1)$. If $(j-Q)/m - a \in \mathbb{Z}$ then $\widehat{p}_j = c_j t^{-1}$ and so in this case

$$p_j(0,t) = c_j t^{(j-Q)/m} \ln(t) + d_j t^{(j-Q)/m} + g(t)\,, \tag{9}$$

$g \in C^\infty(-1,1)$. From (7)–(9) it follows that for any $s \in \mathbb{N}$

$$\Big|U(x,x,t) - \sum_{j=-q(x)}^{s} c_j(x)t^{j/m} - \sum_{j=0}^{s} d_j(x)t^{j/m}\ln(t)\Big| < C_s t^{(s+1)/m}$$

and the proof of Theorem 1 is finished.

From the proof of Theorem 1 one can find the leading coefficient $c_{-q(x)}$ explicitly. It is clear that

$$c_{-q(x)} = v(x) \cdot \int k(0,v,1)\,dv\,,$$

where $v(x) = |\det(\mu_x|_{S(x)})|$ and $k(u,v,t)$ is a fundamental solution for the operator $\widehat{L}$.

For the proof of Theorem 2 we observe that in the Métivier case Θ_x is smooth in $x \in M$ and so the asymptotic formula of Theorem 1 is uniform in x. Consequently, to obtain the statement of Theorem 2 we just integrate this formula over the manifold M.

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