Sharp bounds on heat kernels of higher order uniformly elliptic operators

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1 Introduction

In [D4] Davies established Gaussian heat kernel bounds for a class of higher order elliptic operators with measurable coefficients acting on $L^2(\mathbf{R}^N)$. He considered uniformly elliptic operators of order $2m$ of the general form

$$Hf(x) = \sum_{\substack{|\alpha|\leq m \\ |\beta|\leq m}} (-1)^{|\alpha|} D^\alpha \{a_{\alpha\beta}(x) D^\beta f(x)\} \tag{1}$$

and proved that under certain conditions the kernel $K(t,x,y)$ of the corresponding parabolic equation satisfies an off-diagonal estimate of the form

$$| K(t,x,y) | \leq c_1 t^{-N/2m} \exp\left\{ -c_2 \frac{| x-y |^{2m/(2m-1)}}{t^{1/(2m-1)}} + c_3 t \right\}. \tag{2}$$

Our aim in this paper is to obtain precise quantitative bounds on the constants c_2 and c_3 above in terms of the ellipticity ratio and dimension when the coefficients are measurable. This problem has been well studied in the case $m=1$. Davies [D2] was the first to obtain the optimal constant $c_2 = 1/4$ for uniformly elliptic second order operators with real measurable coefficients, using a Riemannian distance defined in terms of the operator coefficients instead of the Euclidean distance. This result has since been extended in various directions by many different authors and the theory has reached a high level of sophistication. See [D3, R, VSC] for three accounts of that theory.

In the case of higher order operators however, no such bounds on c_2 seem to exist, even if local regularity assumptions on the coefficients are made [R, p441], [K]. We show that the constant c_3 can be taken to be arbitrarily small if the bottom of the L^2 spectrum of H is zero, and that one can put $c_3 = 0$ if H is homogenous. Our main result, Theorem 9, provides an explicit lower bound on c_2 of the stated type. When we apply our method to the simplest case, $H = (-\Delta)^m$, we obtain a value for c_2 which is sharp in one dimension, and which we conjecture is also sharp in higher dimensions. See Theorem 8.

We also consider the difference between short time and long time heat kernel bounds. While the higher order terms dominate for short times, the lower order ones determine the long time estimates; see Proposition 10. The long time behaviour can change dramatically according to whether the lower order part takes negative values or not. Further information on the term $c_3 t$ and long time estimates of heat kernels can be found in [D5].

The method which we follow in this paper is superficially similar to that in [D4]. We still make the assumptions (5) and (9), which were the key estimates of [D4]. However we identify the constant k_λ introduced in Lemma 1 as the crucial quantity involved in the problem, and re-express as many as possible of the estimates of [D4] in terms of that constant. We do this at an abstract level for possible future applications. The value of the results depends both upon obtaining the most efficient possible estimates in terms of k_λ and upon being able to find sharp estimates for k_λ in particular circumstances. We progress towards this in two steps. In Section 4 we give a general form for k_λ which is valid for all homogeneneous operators of order $2m$ acting on $L^2(\mathbf{R}^N)$. We then evaluate k_λ precisely for the particular case $H = (-\Delta)^m$, and use this information to obtain the main theorems of the paper. The fact that the final estimate which we obtain for $H = (-\Delta)^m$ is sharp, clearly indicates the effectiveness of our approach.

2 Preliminary results

If α is a multi-index and x a vector, we use the standard notation D^α and x^α for the partial differential operator $\partial_1^{\alpha_1} \dots \partial_N^{\alpha_N}$ and the number $x_1^{\alpha_1} \dots x_N^{\alpha_N}$ correspondingly.

Let $\Omega \subset \mathbf{R}^N$ be a Euclidean domain. We shall be considering differential operators on $L^2(\Omega)$ of order $2m$ that are comparable to $(-\Delta)^m$ not in the quadratic form sense but in the stronger sense of comparable coefficients. More precisely, let $\{a_{\alpha\beta}(x)\}_{|\alpha|,|\beta| \le m}$ be the uniformly bounded (self-adjoint) complex measurable coefficient matrix of the operator H given by (1). We assume that there exists a positive real constant $\mu \ge 1$ such that

$$\sum_{\substack{|\alpha|=m \\ |\beta|=m}} a_{0,\alpha\beta}\xi_\alpha\bar{\xi}_\beta \le \sum_{\substack{|\alpha|=m \\ |\beta|=m}} a_{\alpha\beta}(x)\xi_\alpha\bar{\xi}_\beta \le \mu \sum_{\substack{|\alpha|=m \\ |\beta|=m}} a_{0,\alpha\beta}\xi_\alpha\bar{\xi}_\beta, \tag{3}$$

for all $x \in \Omega$ and $\xi \in \oplus_{|\alpha|=m}\mathbf{C}$, where the non-negative constant coefficient matrix $A_0 = \{a_{0,\alpha\beta}\}$ is such that

$$\langle(-\Delta)^m f, g\rangle = \int_\Omega \sum_{\substack{|\alpha|=m \\ |\beta|=m}} a_{0,\alpha\beta} D^\alpha f D^\beta \bar{g}\, dx$$

for all functions $f, g \in C_c^\infty(\Omega)$. In the following we denote by c or c_i various constants depending upon m, N and

$$\nu = \sup\{\|a_{\alpha\beta}\|_\infty \quad | \mid \alpha \mid, \mid \beta \mid \le m\} \tag{4}$$

as well as the constant b introduced below.

We point out that it may be the case that zero is an eigenvalue of the matrix A_0; see the example below. Under the above assumptions the operator H is defined to be the self-adjoint operator associated to the closed and symmetric form Q with domain $W_0^{m,2}(\Omega)$ given by

$$Q(f) = \int_\Omega \sum_{\substack{|\alpha|\le m\\ |\beta|\le m}} a_{\alpha\beta}(x) D^\alpha f(x) D^\beta \bar{f}(x)\, dx.$$

We shall call such operators *superelliptic*. Adding a sufficiently large constant to the operator we may assume that Q is positive, and the fact that it is closed is then a consequence of the inequality

$$c^{-1}\|(-\Delta)^{m/2} f\|_2^2 \le Q(f) \le c\left(\|(-\Delta)^{m/2} f)\|_2^2 + \|f\|_2^2\right) \tag{5}$$

which is valid for some $c > 0$ and all $f \in C_c^\infty(\Omega)$.

A superelliptic operator is called *homogeneous* if it is of the special form

$$Hf(x) = \sum_{\substack{|\alpha|=m\\ |\beta|=m}} (-1)^{|\alpha|} D^\alpha\{a_{\alpha\beta}(x) D^\beta f(x)\}.$$

It should be noted that for a given superelliptic operator H the representation (1) is not unique and that different coefficient matrices can induce the same operator. For example, considering the operator Δ^2 on $\mathbf{R}^2$, one can write the expressions

$$\Delta^2 = \partial_{11}^2\partial_{11}^2 + \partial_{22}^2\partial_{22}^2 + \partial_{11}^2\partial_{22}^2 + \partial_{22}^2\partial_{11}^2$$

as well as

$$\Delta^2 = \partial_{11}^2\partial_{11}^2 + \partial_{22}^2\partial_{22}^2 + 2\partial_{12}^2\partial_{12}^2.$$

which relate to the matrices

$$\begin{pmatrix} 1 & 1 & 0\\ 1 & 1 & 0\\ 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 2 \end{pmatrix}$$

correspondingly.

The results in this section apply to any operators satisfying the conditions (5),(9) and (12). In addition to the superelliptic operators defined above we refer to Section 10 of [D4] for another class of 'elliptic' operators of order $2m$ satisfying these conditions. We also note that the only use of the second inequality in (5) is to ensure that the domain of Q is $W_0^{m,2}(\Omega)$, and that all our results can be re-expressed in a slightly more general context; see Proposition 11 below.

Following [D4], we define the class $\mathcal{E}_m = \mathcal{E}_m(\Omega)$ to consist of all bounded real-valued smooth functions ϕ satisfying $\|\nabla\phi\|_\infty \le 1$ and $\|D^\alpha \phi\|_\infty \le b$ for all multi-indices α with $2 \le |\alpha| \le m$, where the positive real number b is fixed throughout the paper.

For $\phi \in \mathcal{E}_m$ and $\lambda \in \mathbf{R}$ the operator acting by multiplication by $e^{\lambda\phi}$ is then a bounded operator on $W_0^{m,2}(\Omega)$. We define the twisted, complex-valued form $Q_{\lambda\phi}$ with domain $W_0^{m,2}(\Omega)$ by

$$Q_{\lambda\phi}(f,g) = Q(e^{\lambda\phi}f, e^{-\lambda\phi}g), \tag{6}$$

so that

$$Q_{\lambda\phi}(f) = \int_\Omega \sum_{\alpha,\beta} a_{\alpha\beta}(x)\{e^{-\lambda\phi}D^\alpha e^{\lambda\phi}f\}\{e^{\lambda\phi}D^\beta e^{-\lambda\phi}\bar{f}\}dx. \tag{7}$$

We also denote the associated operator by $H_{\lambda\phi}$ so that

$$H_{\lambda\phi} = e^{-\lambda\phi}He^{\lambda\phi}. \tag{8}$$

The form $Q_{\lambda\phi} - Q$ is of order $2m-1$, and it is shown in [D4] that

$$| Q_{\lambda\phi}(f) - Q(f) | \leq \epsilon Q(f) + \gamma_\lambda(\epsilon)\|f\|_2^2. \tag{9}$$

for all $0 < \epsilon \leq 1$ and $f \in W_0^{m,2}(\Omega)$, where $\gamma_\lambda(\epsilon)$ is a polynomial of degree $2m$ as a function of $\lambda \in \mathbf{R}$. This is proved by writing an explicit expression for the difference $Q_{\lambda\phi}(f) - Q(f)$ for $f \in C_c^\infty(\mathbf{R}^N)$ and then using estimates of the form

$$\|\lambda^k D^\gamma f\|_2^2 \leq \epsilon\|\nabla^{k+|\gamma|}f\|_2^2 + c\epsilon^{-|\gamma|/k}\lambda^{2k+2|\gamma|}\|f\|_2^2 \tag{10}$$

which are proved by means of the Fourier transform. See [D4] for the proofs of the above statements. We shall see that although ϵ can be taken to be arbitrarily small, what is important is what happens when ϵ is close to one; rather than (9) we shall use the weaker

$$| Q_{\lambda\phi}(f) - Q(f) | \leq \epsilon Q(f) + \gamma_\lambda\|f\|_2^2, \tag{11}$$

valid for all $1/2 \leq \epsilon \leq 1$ and $f \in W_0^{1,2}(\Omega)$.

Before proceeding we note that different $\phi \in \mathcal{E}_m$ may satisfy (12) below for different constants $k_{\lambda,\phi}$. However, (11) implies the crude bound

$$\sup_{\phi\in\mathcal{E}_m} k_{\lambda,\phi} < +\infty.$$

In the rest of this section we shall write simply k_λ instead of $k_{\lambda,\phi}$ and re-introduce the notation $k_{\lambda,\phi}$ in Proposition 4. One has anyway $\sup_{\phi\in\mathcal{E}_m} k_{\lambda,\phi} < +\infty$ for all $\lambda \in \mathbf{R}$.

Lemma 1 *Let $k_\lambda = k_{\lambda,\phi}$ be such that*

$$\mathrm{Re}\ Q_{\lambda\phi}(f) \geq -k_\lambda\|f\|_2^2 \tag{12}$$

for some $\phi \in \mathcal{E}_m$ and all $f \in W_0^{m,2}(\Omega)$. Then

$$\text{(i)} \qquad \|e^{-H_{\lambda\phi}t}\| \leq e^{k_\lambda t}$$

$$\textit{and} \quad \text{(ii)} \qquad \|H_{\lambda\phi}e^{-H_{\lambda\phi}t}\| \leq \frac{c_{r,\epsilon}}{t}e^{(rk_\lambda+\epsilon)t}$$

for all $r > 1$ and $\epsilon > 0$.

Proof : It follows from the method of proof in [D4] that there exists $c > 0$ such that $\gamma_\lambda \leq c(\lambda^{2m} + 1)$ for all $\lambda \in \mathbf{R}$. By looking first at $(-\Delta)^m$ and then at the general case, one also sees that there exists c' such that $k_\lambda \geq c'(\lambda^{2m} - 1)$ for all $\lambda \in \mathbf{R}$. We deduce that there exist constants c_1 and c_2 such that

$$\gamma_\lambda \leq c_1 k_\lambda + c_2 \tag{13}$$

for all $\lambda \in \mathbf{R}$. Now, let $f \in L^2$ and set $f_t = e^{-H_{\lambda\phi}t} f$. Then $f_t \in \mathrm{Dom}(H_{\lambda\phi})$ for all $t > 0$ and

$$\begin{aligned} \frac{d}{dt}\|f_t\|_2^2 &= -\langle H_{\lambda\phi} f_t, f_t\rangle - \langle f_t, H_{\lambda\phi} f_t\rangle \\ &\leq 2k_\lambda \|f_t\|_2^2, \end{aligned}$$

which implies (i).

Now, it follows from (11) that

$$\mathrm{Re}\; Q_{\lambda\phi}(f) \geq \frac{1}{2} Q(f) - \gamma_\lambda \|f\|_2^2 \tag{14}$$

so for $0 \leq \eta \leq 1$ we have

$$\begin{aligned} \mathrm{Re}\; Q_{\lambda\phi}(f) &= (1-\eta)\mathrm{Re}\; Q_{\lambda\phi}(f) + \eta \mathrm{Re}\; Q_{\lambda\phi}(f) \\ &\geq \frac{1-\eta}{2} Q(f) - (1-\eta)\gamma_\lambda \|f\|_2^2 - \eta k_\lambda \|f\|_2^2 \end{aligned} \tag{15}$$

and hence

$$\mathrm{Re}\; \{Q(f) - Q_{\lambda\phi}(f)\} \leq \frac{1+\eta}{2} Q(f) + [(1-\eta)\gamma_\lambda + \eta k_\lambda]\|f\|_2^2.$$

Now, let $f \in L^2(\Omega)$ and $\theta \in (-\pi/2, \pi/2)$ be fixed and for $\rho > 0$ set

$$f_\rho = \exp\{-H_{\lambda\phi}\rho e^{i\theta}\} f.$$

We then have

$$\begin{aligned} \frac{d}{d\rho}\|f_\rho\|_2^2 &= -2\cos\theta\; Q(f_\rho) + 2\mathrm{Re}\; \left[e^{i\theta}(Q - Q_{\lambda\phi})(f_\rho)\right] \\ &= -2\cos\theta\; Q(f_\rho) + 2\cos\theta\; \mathrm{Re}\; [Q(f_\rho) - Q_{\lambda\phi}(f_\rho)] + 2\sin\theta\; \mathrm{Im}\; [Q_{\lambda\phi}(f_\rho)] \\ &\leq -2\cos\theta\; Q(f_\rho) + 2\cos\theta \left\{\frac{1+\eta}{2} Q(f_\rho) + \right. \\ &\qquad \left. +[(1-\eta)\gamma_\lambda + \eta k_\lambda]\|f_\rho\|_2^2\right\} + 2\sin \mid \theta \mid \left\{\frac{1}{2} Q(f_\rho) + \gamma_\lambda \|f_\rho\|_2^2\right\} \\ &= \{(\eta - 1)\cos\theta + \sin \mid \theta \mid\}\, Q(f_\rho) + \\ &\qquad + \{2\cos\theta[(1-\eta)\gamma_\lambda + \eta k_\lambda] + 2\sin \mid \theta \mid \gamma_\lambda\}\, \|f_\rho\|_2^2. \end{aligned}$$

Defining $\alpha \in (0, \pi/2)$ by

$$\tan\alpha = 1 - \eta$$

it follows that for $\mid \theta \mid \leq \alpha$ we have

$$(\eta - 1)\cos\theta + \sin \mid \theta \mid \leq 0$$

and

$$2\cos\theta[(1-\eta)\gamma_\lambda + \eta k_\lambda] + 2\sin \mid \theta \mid \gamma_\lambda \leq 4(1-\eta)\gamma_\lambda + 2k_\lambda.$$

Using (13) we conclude that

$$\frac{d}{d\rho}\|f_\rho\|_2^2 \leq \{4(1-\eta)(c_1 k_\lambda + c_2) + 2k_{mbda}\}\|f_\rho\|_2^2.$$

Solving the differential inequality yields

$$\|f_\rho\|_2 \leq \exp\{2(1-\eta)(c_1 k_\lambda + c_2) + k_\lambda\}\,\|f\|_2,$$

that is,

$$\|e^{-H_{\lambda\phi} z}\| \leq \exp\{[2(1-\eta)(c_1 k_\lambda + c_2) + k_\lambda] \mid z \mid\}$$

for all $\mid \theta \mid \leq \alpha$.

Now, let

$$\tau_{\lambda,\eta} = \frac{2(1-\eta)(c_1 k_\lambda + c_2) + k_\lambda}{\cos\alpha} \tag{16}$$

so that

$$\|e^{-(H_{\lambda\phi} + \tau_{\lambda,\eta})z}\| \leq 1$$

if $\mid \theta \mid \leq \alpha$. It is a known result [D1, p64] that this implies

$$\|(H_{\lambda\phi} + \tau_{\lambda,\eta})e^{-(H_{\lambda\phi}+\tau_{\lambda,\eta})t}\| \leq \frac{c}{\alpha t}.$$

for all $t > 0$. Hence, for any $\delta > 0$ we have

$$\begin{aligned}
\|H_{\lambda\phi}e^{-H_{\lambda\phi}t}\| &\leq \frac{c}{\alpha t}e^{\tau_{\lambda,\eta}t} + \tau_{\lambda,\eta}e^{\tau_{\lambda,\eta}t} \\
&\leq \frac{c}{\alpha t}e^{\tau_{\lambda,\eta}t} + \frac{c_\delta}{t}e^{(1+\delta)\tau_{\lambda,\eta}t} \\
&\leq \frac{c_{\eta,\delta}}{t}e^{(1+\delta)\tau_{\lambda,\eta}t}.
\end{aligned}$$

But it follows from (16) that given $r > 1$ and $\epsilon > 0$ we can find η close enough to one and δ close enough to zero so that

$$(1+\delta)\tau_{\lambda,\eta} \leq r k_\lambda + \epsilon.$$

This proves (ii). $\square$

Hypothesis : At this point a condition on the order $2m$ of the operator is necessary; we assume from now on that $2m > N$.

We shall need the following lemma from [D4]:

Lemma 2 *If $2m > N$ then $f \in W_0^{m,2}(\Omega)$ implies $f \in L^\infty(\Omega)$ and*

$$\|f\|_\infty \leq c\|(-\Delta)^{m/2} f\|_2^{N/2m} \|f\|_2^{1-N/2m}. \tag{17}$$

Moreover, e^{-Ht} is ultracontractive and

$$\|e^{-Ht} f\|_\infty \leq c t^{-N/4m} \|f\|_2 \tag{18}$$

for all $t > 0$ and $f \in L^2$.

Proof : This is proved in [D4] for the case $\Omega = \mathbf{R}^N$; the first estimate then follows for general Ω by using the inclusion $W_0^{m,2}(\Omega) \subset W^{m,2}(\mathbf{R}^N)$. The second then follows as in [D4].

Lemma 3 *The semigroup* $\exp(-H_{\lambda\phi} t)$ *is ultracontractive and*

$$\|e^{-H_{\lambda\phi} t}\|_{\infty,2} \leq c_{r,\epsilon} t^{-N/4m} e^{(rk_\lambda + \epsilon)t}$$

for all $r > 1$ and $\epsilon > 0$.

Proof : Let $f \in L^2$ and set $f_t = e^{-H_{\lambda\phi} t} f$. Using the estimates of the last lemma we have

$$\begin{aligned}
\|f_t\|_\infty &\leq cQ(f_t)^{N/4m} \|f_t\|_2^{1-N/2m} \\
&\leq c\left\{\mathrm{Re}\ Q_{\lambda\phi}(f_t) + \gamma_\lambda \|f_t\|_2^2\right\}^{N/4m} \|f_t\|_2^{1-N/2m} \\
&\leq c\left\{\|H_{\lambda\phi} f_t\|_2 \|f_t\|_2 + (c_1 k_\lambda + c_2)\|f_t\|_2^2\right\}^{N/4m} \|f_t\|_2^{1-N/2m} \\
&\leq c\left\{\frac{c_{r,\epsilon}}{t} e^{(rk_\lambda + \epsilon)t} e^{k_\lambda t} + (c_1 k_\lambda + c_2) e^{2k_\lambda t}\right\}^{N/4m} e^{k_\lambda t(1-N/2m)} \|f\|_2 \\
&= ct^{-N/4m}\{c_{r,\epsilon} e^{(r-1)k_\lambda t + \epsilon t} + (c_1 k_\lambda + c_2)t\}^{N/4m} e^{k_\lambda t} \|f\|_2.
\end{aligned}$$

Given any $r' > 1$ and $\epsilon' > 0$ one can find r close enough one and ϵ close enough to zero so that the last term is smaller than

$$c_{r',\epsilon'} t^{-N/4m} e^{(r' k_\lambda + \epsilon')t} \|f\|_2,$$

as required. $\square$

The starting point for our main theorems will be the following

Proposition 4 *For any $r > 1$ and $\epsilon > 0$ there exists a constant $c_{r,\epsilon}$ such that*

$$| K(t,x,y) | \leq c_{r,\epsilon} t^{-N/2m} \exp\{\lambda(\phi(x) - \phi(y)) + (rk_{\lambda,\phi} + \epsilon)t\}, \tag{19}$$

for all $\lambda \in \mathbf{R}$ and all $\phi \in \mathcal{E}_m$.

Proof : Lemma 3 implies that the kernel $K_{\lambda\phi}(t,x,y)$ of $e^{-H_{\lambda\phi}t}$ satisfies

$$| K_{\lambda\phi}(t,x,y) | \leq c_{r,\epsilon} t^{-N/2m} \exp\{(rk_{\lambda,\phi}+\epsilon)t\}.$$

But it follows from (8) that

$$K_{\lambda\phi}(t,x,y) = e^{-\lambda\phi(x)} K(t,x,y) e^{\lambda\phi(y)},$$

hence

$$| K(t,x,y) | \leq c_{r,\epsilon} t^{-N/2m} \exp\{\lambda(\phi(x)-\phi(y)) + (rk_{\lambda,\phi}+\epsilon)t\} \tag{20}$$

as required. □

3 Linear ϕ's

Up to this point we have taken the function ϕ to lie in $\mathcal{E}_m$. This choice guarantees that the map $f \mapsto e^{\lambda\phi} f$ is a bounded automorphism of $W_0^{m,2}(\Omega)$. Since it is also an automorphism of $L^2(\Omega)$, it induces a canonical functional calculus for the operator $H_{\lambda\phi}$ by the equation

$$f(H_{\lambda\phi}) = e^{-\lambda\phi} f(H) e^{\lambda\phi}. \tag{21}$$

In order to obtain sharp constants below in the case $\Omega = \mathbf{R}^N$, it is necessary to consider functions ϕ that are linear. Since such functions are not bounded some extra arguments are needed; these arguments are unnecessary if the domain Ω is bounded.

Let $\Omega \subset \mathbf{R}^N$ be unbounded and let

$$\phi(x) = a \cdot x$$

where a is a vector of unit length. We cannot use (6) to define $Q_{\lambda\phi}$ since multiplication by $e^{\lambda\phi}$ does not leave $W_0^{m,2}(\Omega)$ invariant. We can however compute the RHS of (7) formally, and a simple calculation yields

$$Q_{\lambda\phi}(f) = \int_\Omega \sum_{\alpha,\beta} a_{\alpha\beta}(x) \sum_{\substack{\gamma_1+\delta_1=\alpha \\ \gamma_2+\delta_2=\beta}} c'_{\gamma_1,\delta_1} c'_{\gamma_2,\delta_2} (\lambda a)^{\gamma_1} (-\lambda a)^{\gamma_2} D^{\delta_1} f D^{\delta_2} \bar{f}\, dx \tag{22}$$

where

$$c'_{\gamma,\delta} = \frac{(\gamma+\delta)!}{\gamma!\,\delta!}.$$

The RHS of (22) is well defined for $f \in W_0^{m,2}(\Omega)$ and we use this formula to define the (closed) form $Q_{\lambda\phi}$. Note that the functional calculus (21) is no longer valid. However, we still have the following

Proposition 5 *Assume $2m > N$ and let k_λ be such that*

$$\mathrm{Re}\, Q_{\lambda\phi}(f) \geq -k_\lambda \|f\|_2^2$$

for some linear function ϕ and all $f \in W_0^{m,2}(\Omega)$. Then

$$| K(t,x,y) | \leq c_{r,\epsilon} t^{-N/2m} \exp\{\lambda(\phi(x)-\phi(y)) + (rk_\lambda + \epsilon)t\}$$

for all $r > 1$ and $\epsilon > 0$.

Proof : Let (Ω_n) be an increasing sequence of bounded domains such that $\cup\Omega_n = \Omega$. For each n we denote by H_n the operator on $L^2(\Omega_n)$ induced by H and satisfying Dirichlet boundary conditions. So H_n is the operator associated to the form Q_n obtained by restricting Q to $W_0^{m,2}(\Omega_n)$. For our given linear ϕ the twisted form $Q_{n,\lambda\phi}$ has already been defined, and we set

$$-k_{\lambda,n} = \inf \mathrm{Re}\, Q_{\lambda\phi}(f)$$

where the infimum is taken over all functions $f \in C_c^\infty(\Omega_n)$ with $\|f\|_2 = 1$. It is immediate that the sequence (k_n) is increasing and that

$$\lim k_{\lambda,n} \leq k_\lambda$$

(with an actual equality holding if k_λ is chosen optimally). Since ϕ is bounded on each Ω_n we can apply our earlier results to the operators H_n and conclude that

$$| K_n(t,x,y) | \leq c_{r,\epsilon} t^{-N/2m} \exp\{\lambda(\phi(x)-\phi(y)) + (rk_{\lambda,n} + \epsilon)t\}$$

for all $r > 1, \epsilon > 0, t > 0$ and $x, y \in \Omega_n$.

Now the sequence Q_n is a decreasing sequence and $Q_n(f) \to Q(f)$ for all $f \in C_c^\infty(\Omega)$. This implies [D3, p8] that

$$(H_n + 1)^{-1} \longrightarrow (H+1)^{-1}$$

strongly (where $(H_n+1)^{-1}$ is now a pseudo-resolvent) and from this follows that

$$e^{-H_n t} \longrightarrow e^{-Ht}$$

strongly, where, again, $e^{-H_n t}$ is interpreted as being zero on $L^2(\Omega \setminus \Omega_n)$ so that its kernel is

$$K_n'(t,x,y) = \chi_{\Omega_n}(x) K_n(t,x,y) \chi_{\Omega_n}(y).$$

For $f, g \in C_c^\infty(\Omega)$ we then have

$$\begin{aligned}
& | \int_{\Omega\times\Omega} K(t,x,y) f(x) g(y) dxdy | \\
= \; & | \langle e^{-Ht} f, g \rangle | \\
= \; & \lim_n | \langle e^{-H_n t} f, g \rangle | \\
= \; & \lim_n | \int_{\Omega_n\times\Omega_n} K_n'(t,x,y) f(x) g(y) dxdy | \\
\leq \; & \limsup_n c_{r,\epsilon} t^{-N/2m} \int_{\Omega_n\times\Omega_n} \exp\{\lambda(\phi(x)-\phi(y)) + (rk_{\lambda,n}+\epsilon)t\} \, | f(x) g(y) | \, dxdy \\
\leq \; & c_{r,\epsilon} t^{-N/2m} \int_{\Omega\times\Omega} \exp\{\lambda(\phi(x)-\phi(y)) + (rk_\lambda+\epsilon)t\} \, | f(x) g(y) | \, dxdy.
\end{aligned}$$

Since f and g are arbitrary, this implies that

$$| K(t,x,y) | \leq c_{r,\epsilon} t^{-N/2m} \exp \{\lambda(\phi(x) - \phi(y)) + (rk_\lambda + \epsilon)t\}$$

as required. $\square$

¿From now on we shall restrict our attention to operators acting on the whole of $\mathbf{R}^N$ and to functions ϕ belonging to the set

$$\mathcal{E}_{lin} =: \{x \mapsto a \cdot x \mid \ a \in \mathbf{R}^N, \ | a | \leq 1\}$$

.

4 Homogeneous operators

In this section we shall consider the case of homogeneous operators and we shall only consider functions $\phi \in \mathcal{E}_{lin}$. In this case every term in (22) has $| \gamma_1 + \delta_1 | = | \gamma_2 + \delta_2 | = m$ and thus it follows from (10) that the function $\gamma_\lambda(\epsilon)$ in (9) can be taken to be of the special form

$$\gamma_\lambda(\epsilon) = \gamma(\epsilon)\lambda^{2m}. \tag{23}$$

Similarly, the estimate (12) can be taken to be of the form

$$\text{Re } Q_{\lambda\phi}(f) \geq -k\lambda^{2m} \|f\|_2^2. \tag{24}$$

The determination of the smallest constant k for which (24) holds is non-trivial and is studied for various particular situations below. We have the following

Lemma 6 *Let $2m > N$ and let H be a homogeneous operator satisfying (24) for all functions $\phi \in \mathcal{E}_{lin}$. We then have*

$$| K(t,x,y) | \leq c_r t^{-N/2m} \exp \left\{ -\frac{2m-1}{2mr} (2km)^{-1/(2m-1)} \frac{| x - y |^{2m/(2m-1)}}{t^{1/(2m-1)}} \right\}$$

for all $r > 1$.

Proof : From Proposition 5 we have

$$| K(t,x,y) | \leq c_{r,\epsilon} t^{-N/2m} \exp \left\{ \lambda(\phi(x) - \phi(y)) + (rk\lambda^{2m} + \epsilon)t \right\}$$

for all $\phi \in \mathcal{E}_{lin}$. Optimizing over all such ϕ yields

$$| K(t,x,y) | \leq c_{r,\epsilon} t^{-N/2m} \exp \left\{ -\lambda | x - y | + (rk\lambda^{2m} + \epsilon)t \right\}$$

and optimizing over λ by putting

$$\lambda = \left(\frac{| x - y |}{2mrkt} \right)^{\frac{1}{2m-1}}$$

yields

$$| K(t,x,y) | \leq c_{r,\epsilon} t^{-N/2m} \exp\left\{ -\frac{2m-1}{2mr}(2km)^{-1/(2m-1)} \frac{| x-y |^{2m/(2m-1)}}{t^{1/(2m-1)}} + \epsilon t \right\}. \tag{25}$$

Using a scaling argument we eliminate the term ϵt: Let $\delta > 0$ be fixed, let U be the unitary operator given by

$$Uf(x) = \delta^{N/2} f(\delta x)$$

and set

$$H' = \delta^{-2m} U^{-1} H U.$$

Then $\{a_{\alpha\beta}(\delta x)\}$ is a coefficient matrix for H' and the heat kernel $K'(t,x,y)$ is related to $K(t,x,y)$ by

$$K(t,x,y) = \delta^N K'(\delta^{2m} t, \delta x, \delta y).$$

Applying (25) to $K'(t,x,y)$ we get

$$\begin{aligned} &| K(t,x,y) | \\ &\quad \leq c_{r,\epsilon} \delta^N (\delta^{2m} t)^{-N/2m} \\ &\qquad \exp\left\{ -\frac{2m-1}{2mr}(2km)^{-1/(2m-1)} \frac{(\delta \mid x-y \mid)^{2m/(2m-1)}}{(\delta^{2m} t)^{1/(2m-1)}} + \epsilon \delta^{2m} t \right\} \\ &\quad = c_{r,\epsilon} t^{-N/2m} \exp\left\{ -\frac{2m-1}{2mr}(2km)^{-1/(2m-1)} \frac{| x-y |^{2m/(2m-1)}}{t^{1/(2m-1)}} + \epsilon \delta^{2m} t \right\}. \end{aligned}$$

The result now follows by letting $\delta \to 0$. □

Powers of the Laplacian

A special case of homogeneous operators that can be treated in more detail is the case where $H = (-\Delta)^m$.

Lemma 7 *Let*

$$k_m = \left(\sin \frac{\pi}{4m-2} \right)^{-(2m-1)}. \tag{26}$$

We have

$$\mathrm{Re}\ Q_{\lambda\phi}(f) \geq -k_m \lambda^{2m} \|f\|_2^2.$$

for all $\phi \in \mathcal{E}_{lin}$ and all $f \in W^{m,2}(\mathbf{R}^N)$.

Proof : Since $\mathrm{Dom}(H_{\lambda\phi})$ is a form core for $Q_{\lambda\phi}$, it is enough to prove that

$$\mathrm{Re}\ \langle H_{\lambda\phi} f, f \rangle \geq -k_m \lambda^{2m} \|f\|_2^2$$

for all $f \in \mathrm{Dom}(H_{\lambda\phi})$. For any multi-indices α, β and γ we set

$$c_\alpha = \frac{(\alpha_1 + \cdots + \alpha_N)!}{\alpha_1! \ldots \alpha_N!}, \qquad c'_{\beta\gamma} = \frac{(\beta+\gamma)!}{\beta!\gamma!}$$

so that

$$\begin{aligned}
\Delta^m(e^{\lambda\phi}f) &= \sum_{|\alpha|=m} c_\alpha D^{2\alpha}(e^{\lambda\phi}f) \\
&= \sum_{|\alpha|=m} c_\alpha \sum_{\beta+\gamma=2\alpha} c'_{\beta\gamma}(D^\gamma e^{\lambda\phi})D^\beta f
\end{aligned}$$

and hence

$$\begin{aligned}
e^{-\lambda\phi}(-\Delta)^m e^{\lambda\phi}f &= (-1)^m {\sum}'(e^{-\lambda\phi}D^\gamma e^{\lambda\phi})D^\beta f \\
&= (-1)^m {\sum}'(\lambda a)^\gamma D^\beta f
\end{aligned}$$

where $\sum' = \sum_{|\alpha|=m} c_\alpha \sum_{\beta+\gamma=2\alpha} c'_{\beta\gamma}$. In the Fourier space this acts by multiplication by the complex-valued polynomial

$$\begin{aligned}
P(\xi) &= (-1)^m {\sum}'(\lambda a)^\gamma (i\xi)^\beta \\
&= (-1)^m \sum_{|\alpha|=m} c_\alpha(\lambda a + i\xi)^{2\alpha} \\
&= (-1)^m\{(\lambda a_1 + i\xi)^2 + \cdots + (\lambda a_N + i\xi_N)^2\}^m \\
&= (\xi^2 - \lambda^2 + 2i\lambda a\cdot\xi)^m \\
&=: \lambda^{2m}\hat{P}(\xi/\lambda)
\end{aligned}$$

where $\hat{P}(\xi) = (\xi^2 + 2ia\cdot\xi - 1)^m$. The minimum of Re $\hat{P}(\xi)$ is attained when $\xi = \mu a$ for an appropriate $\mu \in \mathbf{R}$, and for such a ξ we get

$$P(\xi) = \lambda^{2m}(\mu + i)^{2m}. \tag{27}$$

Writing $\mu + i = re^{i\theta}$ where $r > 0$ and $0 < \theta < \pi$ we have $r^2 = \sin^{-2}\theta$ so that

$$\mathrm{Re}\,(\mu + i)^{2m} = (\sin\theta)^{-2m}\cos 2m\theta.$$

The result follows by minimizing the above with respect to θ. $\square$

The restriction on N in the following theorem is almost surely not necessary.

Theorem 8 *Let $2m > N$ and*

$$\sigma_m = (2m-1)(2m)^{-2m/(2m-1)}\sin(\frac{\pi}{4m-2}).$$

The heat kernel $K(t,x,y)$ of $(-\Delta)^m$ satisfies the bound

$$| K(t,x,y) | \le c_r t^{-N/2m} \exp\left\{ -\sigma_m \frac{| x-y |^{2m/(2m-1)}}{r t^{1/(2m-1)}} \right\} \tag{28}$$

for all $r > 1$.

Proof : Follows from Corollary 4 and Lemma 1. $\square$

Remark The constant σ_m is optimal for $N = 1$ and all m and we conjecture that it is optimal for all values of N and m. First, we have $\sigma_1 = 1/4$, which is known to be optimal. Moreover, in one dimension one can use the tools of asymptotic analysis to find the large x asymptotics of

$$S_m(x) =: K(1, x, 0) = \int_{-\infty}^{\infty} e^{ix\xi - \xi^{2m}} d\xi$$

and one sees that σ_m is optimal. For example, for $m = 2$ the method of steepest descent [F, M] yields

$$S_2(x) \sim 2^{11/6} 3^{-1/2} \pi^{1/2} x^{-2/3} \cos\left(\frac{2^{1/3} 3^{3/2}}{16} x^{4/3} - \frac{\pi}{3} \right) e^{-2^{-11/3} 3 x^{4/3}} \tag{29}$$

as $x \to +\infty$. Since $K(t, x, y) = t^{-1/4} S_2(t^{-1/4}(x - y))$, (29) and a simple argument also show that one cannot put $r = 1$ in (28). Formulas similar to (29) can be established for $m > 2$, but if the dimension is higher, then obtaining an asymptotic estimate becomes much harder. Of course, the method fails completely if one considers operators with variable coefficients.

Variable coefficients

Let H be superelliptic and homogeneous of order $2m$ where $2m > N$. So H has a representation

$$Hf(x) = \sum_{\substack{|\alpha|=m \\ |\beta|=m}} (-1)^{|\alpha|} D^\alpha \{a_{\alpha\beta}(x) D^\beta f(x)\}$$

where the self-adjoint matrix $A(x) = \{a_{\alpha\beta}(x)\}$ is such that

$$A_0 \le A(x) \le \mu A_0 \tag{30}$$

for some constant $\mu \ge 1$ and all $x \in \mathbf{R}^N$, where A_0 is a constant matrix representing the operator $(-\Delta)^m$. This of course implies

$$H_0 \le H \le \mu H_0 \tag{31}$$

in the quadratic form sense.

Theorem 9 *Assume $2m > N$. The kernel $K(t, x, y)$ satisfies the estimate*

$$| K(t, x, y) | \le c_r t^{-N/2m} \exp\left\{ -\rho(\mu, m) \frac{| x - y |^{2m/(2m-1)}}{r t^{1/(2m-1)}} \right\}$$

for all $r > 1$, where

$$\rho(\mu, m) = (2m - 1)(2m)^{-2m/(2m-1)} \mu^{1/(2m-1)} \{k_m + c(\mu - 1)\mu^m\}^{-1/(2m-1)}$$

and k_m is given by (26). In particular

$$\rho(\mu, m) = \sigma_m - O(\mu - 1)$$

as $\mu \to 1$.

Proof : Let $\phi \in \mathcal{E}_{lin}$ and $f \in W^{m,2}$ be fixed. We define the square-integrable vector valued function

$$\{v_{\lambda,\alpha}\}_{|\alpha|=m} = \{e^{-\lambda\phi} D^\alpha e^{\lambda\phi} f(x)\}_{|\alpha|=m},$$

so that by (7)

$$Q_{\lambda\phi}(f) = \int A(x) v_\lambda(x) \cdot v_{-\lambda}(x)\, dx$$

where the dot denotes the standard inner product in $\oplus_{|\alpha|=m}\mathbf{C}$. Writing $\phi(x) = a \cdot x$ we have

$$\begin{aligned} e^{-\lambda\phi} D^\alpha e^{\lambda\phi} f &= \sum_{\gamma+\delta=\alpha} c'_{\gamma,\delta} (e^{-\lambda\phi} D^\gamma e^{\lambda\phi}) D^\delta f \\ &= \sum_{\gamma+\delta=\alpha} c'_{\gamma,\delta} (\lambda a)^\gamma (D^\delta f), \end{aligned}$$

and hence we can write

$$\begin{aligned} v_\lambda &= v_\lambda^+ + v_\lambda^-, \\ v_{-\lambda} &= v_\lambda^+ - v_\lambda^- \end{aligned}$$

where

$$\begin{aligned} v_{\lambda,\alpha}^+ &= \sum_{\substack{\gamma+\delta=\alpha \\ |\gamma| \text{ even}}} c'_{\gamma,\delta} (\lambda a)^\gamma D^\delta f, \\ v_{\lambda,\alpha}^- &= \sum_{\substack{\gamma+\delta=\alpha \\ |\gamma| \text{ odd}}} c'_{\gamma,\delta} (\lambda a)^\gamma D^\delta f. \end{aligned}$$

Thus

$$\begin{aligned} Q_{\lambda\phi}(f) &= \int A v_\lambda \cdot v_{-\lambda}\, dx \\ &= \int A(v_\lambda^+ + v_\lambda^-) \cdot (v_\lambda^+ - v_\lambda^-)\, dx. \end{aligned}$$

Hence from (30) we have

$$\begin{aligned} \text{Re } Q_{\lambda\phi}(f) &= \int (A v_\lambda^+ \cdot v_\lambda^+ - A v_\lambda^- \cdot v_\lambda^-) dx \\ &\geq \int A_0 v_\lambda^+ \cdot v_\lambda^+\, dx - \mu \int A_0 v_\lambda^- \cdot v_\lambda^- dx \\ &= \text{Re } Q_{0,\lambda\phi}(f) - (\mu - 1) \int A_0 v_\lambda^- \cdot v_\lambda^-\, dx \\ &\geq \text{Re } Q_{0,\lambda\phi}(f) - c_0(\mu - 1) \|v_\lambda^-\|_2^2 \end{aligned}$$

where the constant c_0 is independent of ϕ and μ.

The vector v_λ^- only contains derivatives of order $< m$, and it follows from (10) that

$$\|v_\lambda^-\|_2^2 \leq \epsilon Q_0(f) + c\epsilon^{1-m} \lambda^{2m} \|f\|_2^2$$

for all $\epsilon > 0$ and all $f \in W^{m,2}(\mathbf{R}^N)$.

Using the lower bound that we obtained in Lemma 7 for Re $Q_{0,\lambda\phi}$ together with (15) and (23) we have for $0 \leq \eta \leq 1$

$$\begin{aligned} \text{Re } Q_{\lambda\phi}(f) \quad &\geq \quad \{\frac{1-\eta}{2} - c_0(\mu-1)\epsilon\}Q_0(f) - \\ &\quad -\{c(1-\eta) + \eta k_m + c(\mu-1)\epsilon^{1-m}\}\lambda^{2m}\|f\|_2^2 \end{aligned}$$

and taking

$$\epsilon = \frac{1-\eta}{2c_0(\mu-1)}$$

we get

$$\text{Re } Q_{\lambda\phi}(f) \geq -\left\{c(1-\eta) + \eta k_m + c(\mu-1)^m(1-\eta)^{1-m}\right\}\lambda^{2m}\|f\|_2^2.$$

Choosing $\eta \in (0,1)$ so that

$$1-\eta = (\mu-1)/\mu$$

we conclude that

$$\text{Re } Q_{\lambda\phi}(f) \geq -\mu^{-1}\left\{k_m + c(\mu-1)\mu^m\right\}\lambda^{2m}\|f\|_2^2 \tag{32}$$

The result now follows by applying Lemma 6. $\square$

5 Non-homogeneous operators

Up to this point we have only considered homogeneous (in the form sense) operators. One of the common properties of the bounds this far obtained is that they all involve a single term in the exponent, of the general form $c \mid x-y \mid^{2m/(2m-1)} /t^{1/(2m-1)}$. This property is destroyed if one considers non-homogeneous operators.

We shall look at a simple example. Let $m_1 > m_2$ and let

$$H = H_1 + H_2 =: (-\Delta)^{m_1} + (-\Delta)^{m_2}.$$

Note that the heat kernel of H is now of the special form $K(t,x,y) = K_t(x-y)$ and one has

$$K_t = K_{1,t} * K_{2,t} \tag{33}$$

where $K_{i,t}(x-y)$, $i = 1,2$ is the heat kernel of H_i. This however depends on the fact that the operators H_i have constant coefficients. Rather than using (33), we prefer to use the method discussed earlier, which can also be applied in the variable coefficient case. See also the note below.

The off-diagonal behaviour of the heat kernel depends on the ratio $\mid x-y \mid /t$: if the ratio is large (small times) then H_1 is the dominant component; if it very small, then H_2 is. More precisely, let

$$L_r(u) = \inf_{\lambda \in \mathbf{R}} \left\{-\lambda u + r(k_1\lambda^{2m_1} + k_2\lambda^{2m_2})\right\}$$

be the Legendre transform of the function

$$\lambda \mapsto r(k_1\lambda^{2m_1} + k_2\lambda^{2m_2}),$$

which can be computed numerically. We have the following

Proposition 10 *Let $2m_1 > N$. For any $r > 1$ we have*

$$| K(t,x,y) | \leq c_r t^{-N/2m_1} \exp\{tL_r(| x-y | /t)\}.$$

In particular, setting $\rho = (2m_1 - 2m_2)/(2m_2 - 1)$ we have (i) *for large $| x-y | /t$*

$$tL(| x-y | /t) = -\sigma_1 | x-y |^{2m_1/(2m_1-1)} t^{-1/(2m_1-1)} \left(1 - c(| x-y | /t)^{-\rho}\right),$$

and (ii) *for small $| x-y | /t$,*

$$tL(| x-y | /t) = -\sigma_2 | x-y |^{2m_2/(2m_2-1)} t^{-1/(2m_2-1)} (1 - c(| x-y | /t)^{\rho}).$$

Proof : We have from Lemma 7

$$\text{Re } Q_{i,\lambda\phi}(f) \geq -k_i\lambda^{2m_i}\|f\|_2^2, \qquad i = 1,2$$

and hence

$$\text{Re } Q_{\lambda\phi}(f) \geq -\left(k_1\lambda^{2m_1} + k_2\lambda^{2m_2}\right)\|f\|_2^2.$$

Hence, by Lemma 4 we obtain a pointwise bound on the kernel of the corresponding semigroup

$$| K(t,x,y) | \leq c_r t^{-N/2m_1} \exp(rA_{r,\lambda}), \qquad \text{all } r > 1, \tag{34}$$

where

$$A_{r,\lambda} = -\lambda | x-y | + r(k_1\lambda^{2m_1} + k_2\lambda^{2m_2})t,$$

and the first assertion follows by taking the infimum over λ.

As for the two asymptotic estimates, the first one follows from (34) by choosing

$$\lambda = \left[(2m_1k_1)^{-1} | x-y | t^{-1}\right]^{1/(2m_1)}$$

while the dual choice proves the second. $\square$

The same arguments can be used to obtained similar bounds when one considers the sum of general homogeneous operators with variable coefficients. The expression in the exponential will then involve some extra terms, namely the lower bounds on Re $Q_{\lambda\phi}$ that were obtained in the proof of Theorem 9. We do not pursue the details.

As one would expect, adding a non-negative potential to an operator does not pose any problems for heat kernel estimates. Let H_0 be a general superelliptic operator (not necessarily homogeneous). Given a non-negative potential $V \in L^1_{\text{loc}}(\mathbf{R}^N)$, one can define $H = H_0 + V$ to be the operator associated to the (closed) form Q defined by

$$\mathrm{Dom}(Q) = \{f \in \mathrm{Dom}(Q_0) \ \mid \int V \mid f \mid^2 dx < +\infty\}$$

and

$$Q(f) = Q_0(f) + \int V \mid f \mid^2 dx, \qquad f \in \mathrm{Dom}(Q).$$

Although $\mathrm{Dom}(Q)$ does not necessarily coincide with $W^{m,2}$, the theory still applies. Estimate (9) is valid since $Q_{\lambda\phi} - Q = Q_{0,\lambda\phi} - Q_0$, and although the second inequality in (5) no longer holds, one easily checks that this is not a problem and that the proofs of Lemmas 1-3 are still valid. Hence we have

Proposition 11 *Any heat kernel bound obtained for H_0 by means of Proposition 4 is also valid for H.*

Proof : By hypothesis, we have an estimate on $Q_{0,\lambda\phi}$ of the form

$$\mathrm{Re}\ Q_{0,\lambda\phi}(f) \geq -k_\lambda \|f\|_2^2.$$

Hence

$$\begin{aligned} \mathrm{Re}\ Q_{\lambda\phi}(f) &= \mathrm{Re}\ Q_{0,\lambda\phi}(f) + \int V \mid f \mid^2 \ dx \\ &\geq -k\|f\|_2^2 \end{aligned}$$

and the result follows from Lemma 4. $\square$

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