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**Heat Kernel Bounds for  
Higher Order Elliptic Operators**

**E B Davies**

## 1. Introduction

We discuss the following questions for self-adjoint, non-negative, elliptic operators  $H$  acting on  $L^2(\mathbf{R}^N)$ .

- (i) For what values of  $p \neq 2$  can the Cauchy problem  $f'(t) = -Hf(t)$  be solved in  $L^p$  for arbitrary initial data in  $L^p$  ?
- (ii) When is the solution to the Cauchy problem in  $L^2$  associated with a heat kernel which satisfies ‘Gaussian’ upper bounds?
- (iii) For what values of  $p \in [1, \infty]$  is the spectrum of  $H$  in  $L^p$  independent of  $p$  ?

Those familiar only with the theory of second order elliptic operators with real coefficients or with the properties of Schrödinger operators whose potentials lie in the Kato class might be forgiven for thinking that almost everything possible has already been said about this problem, [D2, Si2, VSC]. However there has been a great shift in our understanding over the last three years for classes of operators which differ from the above only slightly. We discuss three different developments of the theory which are linked by the fact that they involve similar techniques and lead to similar answers to the above questions. Specifically we discuss second order uniformly elliptic operators with measurable complex coefficients, higher order uniformly elliptic operators whose highest order coefficients are measurable, and Schrödinger operators for which the potential is not Kato class but satisfies a quadratic form bound with respect to  $-\Delta$  with relative bound less than 1. In all of these cases we find that the theory is dependent upon the space dimension in a manner which does not occur for the more standard classes of elliptic operators.

## 2. Second Order Operators

We start with a short review of some standard results concerning heat kernel bounds for second order uniformly elliptic operators with real coefficients. Throughout the paper the word ‘elliptic’ is taken to include the assumption that the operator is given in divergence form; see (1) and (2).

Let  $H = H^* \geq 0$  be the self-adjoint operator on  $L^2(\mathbf{R}^N)$  given formally by

$$Hf(x) := - \sum_{i,j=1}^N \frac{\partial}{\partial x_i} \left\{ a_{i,j}(x) \frac{\partial f}{\partial x_j} \right\} \quad (1)$$

where the coefficients  $a_{i,j}(x)$  are assumed to be real, symmetric, measurable and uniformly elliptic. Since the domain of this operator may not contain  $C_c^\infty$ , we define it rigorously to be the self-adjoint operator associated with the closed quadratic form defined on  $W^{1,2}$  by

$$Q(f, g) := \int_{\mathbf{R}^N} \sum_{i,j=1}^N a_{i,j}(x) \frac{\partial f}{\partial x_j} \frac{\partial \bar{g}}{\partial x_i} d^N x.$$

In 1968 Aronson [Aro] proved that the heat kernel  $K(t, x, y)$  associated with  $H$  satisfies the upper and lower bounds

$$c_1 t^{-N/2} \exp[-c_2 d(x, y)^2/t] \leq K(t, x, y) \leq c_3 t^{-N/2} \exp[-c_4 d(x, y)^2/t]$$

for certain undetermined positive constants  $c_i$  and all  $t > 0$  and  $x, y \in \mathbf{R}^N$ . In this bound  $d(x, y)$  denotes the Euclidean distance between  $x$  and  $y$ . Davies [D] used a quite different method to show that one can take  $c_4$  as close to  $1/4$  as one likes if one defines  $d(x, y)$  to be a certain Riemannian distance constructed using the coefficients of the operator. This method was rapidly extended to a variety of other second order elliptic operators, including Laplace-Beltrami operators on complete Riemannian manifolds, and there are now excellent reviews of progress in this area [D2, R, VSC]. We should also mention that Aronson type upper and lower bounds hold for a Schrödinger operator  $H := -\Delta + V$  acting on  $L^2(\mathbf{R}^N)$  if  $0 < t < 1$  and the potential  $V$  lies in the Kato class, [Si2].

Any changes in the hypotheses invalidate the above results. If one assumes that the coefficient matrix is complex, measurable, and uniformly elliptic, then the heat kernel is not real-valued, so one cannot even discuss lower bounds. More seriously, for complex coefficients it is only known how to prove a Gaussian upper bound on the absolute value of the heat kernel in the case if  $N = 1$  or  $N = 2$ , [AMT]. There are certainly fundamental differences in the theory if  $N \geq 5$ , [Au, MNP], and probably for all  $N \geq 3$ .

### 3. Higher Order Operators

When one turns to higher order elliptic operators one finds a number of differences from the behaviour of second order operators even for operators with constant coefficients. Although the biharmonic operator on the unit square in  $\mathbf{R}^2$  subject to Dirichlet boundary conditions has compact resolvent, its Green function is not positive, and the ground state eigenfunction is not positive either; this was first discovered numerically [BR] and later proved analytically [C, KKM]. The same behaviour occurs for a clamped circular plate with a sufficiently small central hole, [CD].

On the other hand when one studies spectral asymptotics, there is a large body of results for elliptic operators of arbitrary order. We mention particularly [VG] because of its comparison of the two term spectral asymptotics of a variety of thin elastic shells with numerical calculations of their first hundred eigenvalues.

We refer to [PV2] for the large literature concerning the solution of the Dirichlet problem with  $L^p$  boundary data for the operator  $(-\Delta)^m$ ; the results obtained are heavily dependent upon  $m$  and the dimension of the underlying space. We refer to [PV1] for references to the literature concerning the maximum principle for the biharmonic operator in Lipschitz domains; once again the dimension of the underlying space is crucial. We finally mention that given a constant coefficient fourth order elliptic operator  $H = H^* \geq 0$  on  $L^2(\mathbf{R}^N)$ , one cannot assume that the semigroup  $t \rightarrow e^{-Ht}$  is uniformly bounded in norm on  $L^1(\mathbf{R}^N)$ ; a counterexample is given in [D6].

We now turn to the study of the heat kernels of higher order self-adjoint elliptic operators acting on  $L^2(\mathbf{R}^N)$ . Our main interest is in the case in which the highest order coefficients are measurable, a possibility excluded by most of the existing literature. The initial motivation for the analysis in [D5] was a desire to be able to handle the vibrations of elastic bodies with inhomogeneous, possible random, mass distributions. Before continuing we mention that the theory described below has been set in a Riemannian manifold context in [D5], but we only describe the Euclidean version here.

Let  $\alpha, \beta$  denote multi-indices of the usual type, and  $D^\alpha$  the corresponding partial differentiation operators. We consider the higher order analogue of (1), namely the symmetric operator given formally by

$$Hf(x) := \sum_{\substack{|\alpha| \leq m \\ |\beta| \leq m}} (-1)^{|\alpha|} D^\alpha \{ a_{\alpha,\beta}(x) D^\beta f(x) \} \quad (2)$$

where  $a_{\alpha,\beta}(x) = \overline{a_{\beta,\alpha}(x)}$  are complex-valued bounded measurable functions on  $\mathbf{R}^N$  for all  $\alpha, \beta$ . It is clear that  $\mathbf{C}_c^\infty$  need not be contained in the domain of such operators. We therefore start from the quadratic form  $Q$  defined on  $W^{m,2}$  by

$$Q(f, g) := \int_{\mathbf{R}^N} \sum_{\substack{|\alpha| \leq m \\ |\beta| \leq m}} a_{\alpha,\beta}(x) D^\beta f(x) \overline{D^\alpha g(x)} d^N x.$$

We make suitable assumptions on the highest order coefficients, those for which  $|\alpha| = |\beta| = m$ , to ensure that after adding a suitable constant to the operator, one has the

Gårding inequality

$$c^{-1}Q_0(f) \leq Q(f) \leq cQ_0(f) + c\|f\|_2^2 \quad (3)$$

for some  $c > 0$  and all  $f \in W^{m,2}$ , where  $Q(f) := Q(f, f)$ , and

$$Q_0(f) := \int_{\mathbf{R}^N} |\nabla f|^{2m} d^N x.$$

Our second condition involves bounds on a twisted form which is defined in terms of a certain class of multipliers. Let  $\mathcal{E}_m$  denote the set of all bounded real-valued  $C^\infty$  functions  $\phi$  on  $\mathbf{R}^N$  such that  $\|D^\alpha \phi\|_\infty \leq 1$  for all  $\alpha$  such that  $1 \leq |\alpha| \leq m$ . We make no assumption on the size of  $\|\phi\|_\infty$ . Given  $\lambda \in \mathbf{R}$  and  $\phi \in \mathcal{E}_m$  the functions  $e^{\lambda\phi}$  may be regarded as bounded invertible multiplication operators on  $L^2$  and also on  $W^{m,2}$ . We define the complex-valued form  $Q_{\lambda\phi}$  by

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

for all  $f \in W^{m,2}$ . For operators  $H$  defined in the above manner it may be shown that

$$|Q_{\lambda\phi}(f) - Q(f)| \leq bQ(f) + k(1 + \lambda^{2m})\|f\|_2^2 \quad (4)$$

for some  $k \geq 0$ ,  $0 < b < 1$  and all  $f \in W^{m,2}$ . We remark that it is possible to base an abstract theory upon the hypotheses (3) and (4), and this enables one to treat a rather larger class of elliptic operators of order  $2m$  than those described by (2).

**LEMMA 1.** *Let  $E$  and  $F$  be disjoint compact convex sets in  $\mathbf{R}^N$  and put*

$$d(E, F) := \min\{|x - y| : x \in E, y \in F\}.$$

*There exist positive constants  $c_1, c_2$  such that*

$$\|P_E e^{-Ht} P_F\| \leq \exp \left[ -c_1 d(E, F)^{2m/(2m-1)} t^{-1/(2m-1)} + c_2 t \right]$$

for all  $t > 0$ .

Proof We use (4) to obtain a lower bound on the self-adjoint part of  $e^{\lambda\phi} H e^{-\lambda\phi}$ , and then a differential inequality to obtain an upper bound on the  $L^2$  operator norms of  $e^{\lambda\phi} e^{-Ht} e^{-\lambda\phi}$  for  $t \geq 0$ . The result is then completed by choosing  $\lambda$  and  $\phi$  optimally, having regard to the particular choice of  $E$  and  $F$ .

This is the key result for subsequent analysis. The  $L^2$  Gaussian off-diagonal decay which it yields has now to be converted to pointwise off-diagonal decay. Unlike the situation with second order operators, this is not always possible. We can certainly prove pointwise off-diagonal decay if  $N < 2m$ , and conjecture that  $N \leq 2m$  is the weakest condition for such results, unless one imposes some type of local regularity condition on the highest order coefficients. The point of the condition  $N < 2m$  is that it implies that the quadratic form domain of  $H$  consists entirely of bounded continuous functions, by a standard Sobolev embedding theorem.

**THEOREM 2.** If  $N < 2m$  then there exist positive constants  $c_1$ ,  $c_2$  and  $c_3$  such that

$$|K(t, x, y)| \leq c_1 t^{-N/2m} \exp[-c_2|x - y|^{2m/(2m-1)} t^{-1/(2m-1)} + c_3 t] \quad (5)$$

for all  $t > 0$  and  $x, y \in \mathbf{R}^N$ .

Bounds of this type are not new if one assumes that the highest order coefficients are smooth [ER, K, R], and the point is that we only assume measurability of the highest order coefficients. The precise values of the constants in this theorem were not determined in [D5], and are apparently not known even for the case of smooth coefficients [ER, K, R]. In a forthcoming paper with Barbatis [BD], we show that the constant  $c_3$  can be taken arbitrarily small, and can be put equal to 0 if  $H$  is homogeneous, that is if one only has terms with  $|\alpha| = |\beta| = m$  in (2). We also obtain an explicit expression for  $c_2$  as a function of  $N$ ,  $m$  and the ellipticity constant of  $H$ . When applied to  $H_0 := (-\Delta)^m$ , we obtain the value

$$c_2 = r^{-1} (2m-1) (2m)^{-2m/(2m-1)} \sin\left(\frac{\pi}{4m-2}\right)$$

which is sharp in one dimension, and probably in any dimension, apart from the factor  $r > 1$ , which may be as close to 1 as one cares.

**THEOREM 3.** If  $N < 2m$  then the operators  $e^{-Hz}$  on  $L^2$  may be extended to bounded operators  $T_p(z)$  on  $L^p$  satisfying

$$\|T_p(z)\| \leq c(\cos \theta)^{-2N|\frac{1}{p} - \frac{1}{2}|} e^{kr \cos \theta} \quad (6)$$

for all  $1 \leq p \leq \infty$  and all  $z = re^{i\theta}$  such that  $r > 0$  and  $|\theta| < \frac{\pi}{2}$ .

The fact that the angle of holomorphicity is  $\pi/2$  was first proved for second order elliptic operators by Ouhabaz [O], and is crucial for the applications below.

Proof One first extends the bound (5) of the last theorem to all complex times  $t$  such that  $\operatorname{Re}(t) > 0$  by a standard complex variable technique. The  $L^1$  operator norms can then be estimated directly from the bounds on the integral kernels. For other values of  $p$  one deduces the result by duality and interpolation.

If  $N \geq 2m$  then a similar operator norm bound may be proved for  $p$  in a certain interval around  $p = 2$ , even though we then have no pointwise heat kernel bounds [D5].

#### 4. $L^p$ Spectral Theory

We start by considering the  $L^p$  spectral theory of Schrödinger operators  $H := -\Delta + V$  acting on  $L^2(\mathbf{R}^N)$ . The proof of  $L^p$  spectral independence for Schrödinger operators with Kato potentials was given by Hempel and Voigt [HV]. If one only assumes that the potential satisfies a quadratic form bound relative to  $H$  with constant less than 1 then it is known that one only has a good  $L^p$  theory for  $p$  in an interval around  $p = 2$ , [D5, SV]. A complete analysis of the range of values of  $p$  for which the semigroup  $e^{-Ht}$  acts on  $L^p$  and for which the  $L^p$  spectrum of  $H$  is independent of  $p$  has recently been given by Semenov [Se].

More generally, Arendt [Are] showed in a Euclidean space context that the proof of [HV] for second order elliptic operators depends only upon the existence of suitable Gaussian upper bounds on the absolute value of the heat kernel. It is worth mentioning that  $L^p$  spectral independence is not a universal fact. If we return to the study of Laplace-Beltrami operators on complete Riemannian manifolds, it is possible to give geometrical conditions for this property. Sturm [St] has shown that if the volumes of balls are bounded uniformly subexponentially as the radius diverges to infinity, then the  $L^p$  spectrum is independent of  $p$ . On the other hand it is known [DM, DST] that the  $L^p$  spectrum of hyperbolic space and other non-compact hyperbolic manifolds does depend on  $p$ , and that it is not even real unless  $p = 2$ . Of course the volumes of large balls in hyperbolic space grow exponentially. Another approach to the proof of  $L^p$  spectral independence based upon the Helffer-Sjöstrand formula, discussed below, has been given by the author in a context which allows application to systems and to Schrödinger operators with magnetic fields [D3, D4]. The method yields a slightly weaker result than that of Sturm for Laplace-Beltrami operators, but may also be applied to higher order elliptic operators [D5]:

**THEOREM 4.** *Let  $N < 2m$  and let  $-H_p$  be the generator of the holomorphic semigroup  $T_p(z)$  on  $L^p$ . Then the spectrum of  $H_p$  is independent of  $p$  for  $1 \leq p < \infty$ . A similar result holds for  $N \geq 2m$  in a certain open interval around  $p = 2$ .*

Proof One first obtains  $L^p$  operator bounds on the resolvent operators, by estimating suitable integrals involving the heat semigroups. If  $\text{Re}(z) < 0$  one may use (6) and

$$(z - H)^{-1} = - \int_0^\infty e^{-Ht} e^{zt} dt$$

and for other  $z \notin \mathbf{R}$  one employs a related complex time contour integral. From these calculations we learn that the spectrum of  $H_p$  is real for all  $1 \leq p < \infty$  and that

$$\|(z - H_p)^{-1}\| \leq c |\text{Im}z|^{-1} \left( \frac{\langle z \rangle}{|\text{Im}z|} \right)^\alpha \quad (7)$$

for some  $\alpha \geq 0$  and all  $z \notin \mathbf{R}$ , where  $\langle z \rangle := (1 + |z|^2)^{1/2}$ . The values of  $\alpha$  and  $c$  obtained in this way depend upon  $p$  and are not optimal, but this does not matter for our purposes. We mention that for Schrödinger operators resolvent bounds of the

form (7) have been studied by Pang [P] and Jensen and Nakamura [JN1, JN2], the latter in the context of scattering theory.

From this point on we use an abstract functional analytic argument which depends only upon the existence of the estimates (7), and therefore drop explicit reference to the value of  $p$ . The key to the proof is the use of the Helffer-Sjöstrand formula [HS]:

$$f(H) := -\frac{1}{\pi} \int_{\mathbf{C}} \frac{\partial \tilde{f}}{\partial \bar{z}} (z - H)^{-1} dx dy$$

valid for all  $f : \mathbf{R} \rightarrow \mathbf{C}$  in a certain algebra containing  $C_c^\infty(\mathbf{R})$ . In this formula  $\tilde{f}$  is an almost analytic extension of  $f$  to the complex plane, and lies in  $C^\infty(\mathbf{C})$ . The notion of almost analytic extension is due to Hörmander [Hö], and for our purposes it suffices to use the explicit formula

$$\tilde{f}(x, y) := \left( \sum_{r=0}^n f^{(r)}(x) (iy)^r / r! \right) \sigma(x, y)$$

where

$$\sigma(x, y) := \tau(y/\langle x \rangle)$$

and  $\tau$  is a non-negative  $C^\infty$  function such that  $\tau(s) = 1$  if  $|s| \leq 1$  and  $\tau(s) = 0$  if  $|s| \geq 2$ . It is shown in [D3] that the bounded operator  $f(H)$  is independent of the choice of  $n$  and of the cut-off function  $\tau$ , provided  $n$  is large enough, depending upon  $\alpha$ . The integral is norm convergent even though the resolvent norm diverges as one approaches the real axis. The H-S formula actually defines a functional calculus on the  $L^p$  spaces; in other words the map  $f \rightarrow f(H_p)$  is a bounded algebra homomorphism from a certain algebra of functions on  $\mathbf{R}$  to the algebra of bounded linear operators on  $L^p$ , [D3]. The functional calculus acts consistently for different values of  $p \in [1, \infty]$  in an obvious sense. The final step uses the consistency of the functional calculi and the fact that if  $x \in \mathbf{R}$  then  $x \notin \text{Spec}(H_p)$  if and only if there exists  $f \in C_c^\infty$  such that  $f(x) \neq 0$  but  $f(H_p) = 0$ , [D4].

## 5. Spectral Theory in Other Banach Spaces

There is no reason to confine attention to the action of the semigroup  $e^{-Ht}$  on the  $L^p$  spaces. One can study the spectral behaviour of  $H$  on a variety of other spaces, such as polynomially weighted  $L^p$  spaces, [D4]. At the abstract level the key issue is whether one can prove a resolvent estimate of the form of (7). It is particularly useful to distinguish between the local regularisation and global off-diagonal decay properties of the semigroup, since the former depends upon the space dimension while the latter does not. This is achieved as follows.

The spaces  $l^p(L^2)$  are defined for  $1 \leq p < \infty$  as follows [BS, Si1]. Given  $m \in \mathbf{Z}^N$  let  $C_m$  be the cube with centre  $m$  and edges oriented parallel to the axes and of length 1. If  $f \in L_{\text{loc}}^2$  and  $1 \leq p < \infty$  we say that  $f \in l^p(L^2)$  if the norm

$$\|f\|_{p,2} := \left( \sum_{m \in \mathbf{Z}^N} \|f|_{C_m}\|_2^p \right)^{1/p}$$

is finite. The definition of  $l^\infty(L^2)$  is similar. Clearly  $l^2(L^2) = L^2$  and  $l^p(L^2) \subseteq L^2$  if  $1 \leq p \leq 2$ . Moreover  $l^p(L^2)^* = l^q(L^2)$  in a natural sense if  $1 \leq p < \infty$  and  $p^{-1} + q^{-1} = 1$ .

We emphasise that the following theorem is valid for all  $m \geq 1$  and  $N \geq 1$ .

**THEOREM 5.** *The semigroup  $e^{-Hz}$  defined for all  $z \in \mathbf{C}$  such that  $\text{Re } z > 0$  restricts (resp. extends) to a holomorphic semigroup  $T_p(z)$  on  $l^p(L^2)$  if  $1 \leq p < 2$  (resp.  $2 < p < \infty$ ). The generator  $-H_p$  of the induced semigroup has spectrum independent of  $p$  in the same range.*

We refer to [D5] for the proof.

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