

GAUSSIAN UPPER BOUNDS ON HEAT KERNELS OF UNIFORMLY ELLIPTIC OPERATORS ON BOUNDED DOMAINS

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*Dedicated to Papa Ji, my grandfather, Sardar Nachhattar Singh Claire who left us on the
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ABSTRACT. We obtain Gaussian upper bounds for heat kernels of higher order differential operators with Dirichlet boundary conditions on bounded domains in \mathbb{R}^N . The bounds exhibit explicitly the nature of the spatial decay of the heat kernel close to the boundary as well as the long-time exponential decay implied by the spectral gap. We make no smoothness assumptions on our operator coefficients which we assume only to be bounded and measurable.

KEYWORDS: *Heat kernel, parabolic, uniformly elliptic, gaussian bounds.*

MSC (2000): Primary 35K25; Secondary 35K08, 47F05, 35P05.

INTRODUCTION

Off-diagonal Gaussian upper bounds for higher order differential operators with bounded measurable coefficients were first obtained by Davies [4]. The operators considered in that exposition were of order $2m$ on $L^2(\mathbb{R}^N)$ with $2m > N$. The higher order operators, expressed as:

$$(0.1) \quad Hf(x) := \sum_{|\alpha| \leq m, |\beta| \leq m} (-1)^{|\alpha|} D^\alpha (a_{\alpha, \beta}(x) D^\beta f(x))$$

were shown to have heat kernels with off-diagonal bounds demonstrated in the inequality:

$$(0.2) \quad |k(t, x, y)| \leq c_1 t^{-N/2m} \exp \left(-c_2 \frac{|x-y|^{2m/(2m-1)}}{t^{1/(2m-1)}} + c_3 t \right).$$

Subsequently Barbatis and Davies [2] were able to obtain optimal values for the constants c_2 and c_3 in terms of the ellipticity ratio and dimension.

In this paper we address the question of upper bounds on heat kernels generated by uniformly elliptic differential operators with Dirichlet boundary conditions on bounded regions of \mathbb{R}^N . We make the same assumptions of the coefficients as in [4], namely that they are measurable and bounded, and consequently find it more convenient to carry out the analysis with greater focus on the corresponding quadratic forms. We do however assume that the quadratic forms, on a bounded region $\Omega \subset \mathbb{R}^N$, satisfy the ellipticity condition:

$$c^{-1} \|(-\Delta)^{m/2} f\|_2^2 \leq Q(f) \leq c \|(-\Delta)^{m/2} f\|_2^2$$

for each $f \in C_c^\infty(\Omega)$ and c strictly positive.

Although estimate (0.2) holds for operators on bounded regions with Dirichlet boundary conditions, the bounds do not reflect either the spatial decay near the boundary or the long-time asymptotics. We extract the manner in which

$$k(t, x, y) \rightarrow 0 \quad \text{as } x, y \rightarrow \partial\Omega$$

and show that the heat kernel has off-diagonal bounds demonstrated in the inequality:

$$|k(t, x, y)| \leq c_1 \left(1 - \frac{N + 2\gamma}{2m}\right)^{-1} t^{-(N+2\gamma)/2m} d(x, \partial\Omega)^\gamma d(y, \partial\Omega)^\gamma \\ \exp\left(-c_2 \frac{|x - y|^{2m/(2m-1)}}{t^{1/(2m-1)}} - st\right)$$

where $0 \leq \gamma < m - N/2$ and s is the spectral gap.

The techniques we employ are close to those employed in [4], but we give more emphasis to the analysis of spatial derivatives of the heat kernel. Moreover the exponential time decay is deduced by exploiting the spectral gap.

Sharp off diagonal heat kernel bounds were also obtained by Barbatis [1] in terms of a non-euclidean metric based on the coefficients of the operator, replacing the term $|x - y|$ in (0.2) by $d(x, y)$. In the case of bounded regions, an off diagonal bound was obtained for highly non-convex regions for the uniformly elliptic operator by Owen [6], in which he used the geodesic distance but boundary behaviour was not the focus of that analysis.

Throughout this paper we will assume that c and c_i represent strictly positive constants.

1. NOTATION

Given $\alpha \in \mathbb{R}^N$ representing the multi-index $(\alpha_1, \alpha_2, \alpha_3, \dots)$ where

$$|\alpha| := \alpha_1 + \alpha_2 + \alpha_3 + \dots + \alpha_N$$

we define the corresponding operator

$$D^\alpha f := \frac{\partial^{|\alpha|} f}{\partial^{\alpha_1} x_1 \partial^{\alpha_2} x_2 \partial^{\alpha_3} x_3 \dots \partial^{\alpha_N} x_N}$$

and the set V_α such that

$$V_\alpha = \{\mathbf{r} : r_i \leq \alpha_i \text{ for all } i\}.$$

Moreover given any multi-index \mathbf{r} in V_α we define the vector factorial as

$$\binom{\alpha}{\mathbf{r}} := \binom{\alpha_1}{r_1} \binom{\alpha_2}{r_2} \binom{\alpha_3}{r_3} \cdots \binom{\alpha_N}{r_N}.$$

The directional derivative of order m of an appropriately smooth function along a vector \mathbf{v} in \mathbb{R}^N is expressed as

$$\frac{\partial^m f}{\partial \mathbf{v}^m} := \cdots \nabla (\nabla (\nabla f \cdot \mathbf{v}) \cdot \mathbf{v}) \cdot \mathbf{v}.$$

2. QUADRATIC FORM

It is helpful to give an indicative though a non-rigorous formulation of the family of higher order operators that we focus on in this paper. The operator is defined more completely through its quadratic form. Given a bounded domain Ω in \mathbb{R}^N we express the operator of order $2m > N$ as

$$(2.1) \quad Hf(\mathbf{x}) := \sum_{|\alpha| \leq m, |\beta| \leq m} (-1)^{|\alpha|} D^\alpha (a_{\alpha, \beta}(\mathbf{x}) D^\beta f(\mathbf{x}))$$

where $a_{\alpha, \beta}$ are complex bounded measurable functions. The associated quadratic form Q

$$(2.2) \quad Q(f) := \sum_{|\alpha| \leq m, |\beta| \leq m} \int_{\Omega} a_{\alpha, \beta}(\mathbf{x}) D^\beta f(\mathbf{x}) \overline{D^\alpha f(\mathbf{x})}$$

defined with domain equal to the Sobolev space $W_0^{m,2}(\Omega)$ will be assumed to satisfy the ellipticity condition with a strictly positive constant c

$$(2.3) \quad c^{-1} \|(-\Delta)^{m/2} f\|_2^2 \leq Q(f) \leq c \|(-\Delta)^{m/2} f\|_2^2.$$

We define the spectral gap

$$s = \inf_{f \in C_c^\infty(\Omega)} \frac{Q(f)}{\|f\|_2^2}.$$

Since we have made the assumption that $N/2m < 1$, it will be informative to track the dependency on this constraint by defining the quantity $0 < \varepsilon \leq 1 - N/2m$ and

$$\gamma := m(1 - \varepsilon) - \frac{N}{2}.$$

For a given point x in Ω we define its distance from the boundary $\partial\Omega$

$$d_x := d(x, \partial\Omega) = \inf_{\mathbf{y} \in \partial\Omega} |\mathbf{x} - \mathbf{y}|.$$

We define the function $\tilde{g}(t)$ such that

$$(2.4) \quad \tilde{g}(t) := \begin{cases} se^{-2st} & t > \frac{1}{s}, \\ \frac{1}{t}e^{-st-1} & t \leq \frac{1}{s}. \end{cases}$$

3. BOUNDARY BEHAVIOUR

Having imposed Dirichlet boundary conditions on our operator we expect the heat kernel $k(t, x, y)$ to vanish at the boundary. The precise nature of this decay can be deduced by application of the Sobolev embedding theorem:

$$W_0^{m,2}(\Omega) \hookrightarrow C_0^\gamma(\Omega).$$

We consider the norm on $C_0^\gamma(\Omega)$ to be defined as

$$\|f\|_{C_0^\gamma} := \sum_{|\alpha| \leq n} \|D^\alpha f\|_\infty + \sup_{x, y \in \Omega} \frac{|D^\alpha f(y) - D^\alpha f(x)|}{|y - x|^\kappa}$$

where n and κ are the integer and the fractional parts of γ respectively.

LEMMA 3.1. *There is a strictly positive constant c such that for all $f \in W_0^{m,2}(\Omega)$ and any unit vector v in \mathbb{R}^N*

$$(3.1) \quad \left| \frac{\partial^n f(x)}{\partial v^n} \right| \leq \frac{c}{\sqrt{\varepsilon}} d_x^\kappa Q(f)^{(1-\varepsilon)/2} \|f\|_2^\varepsilon$$

for all $x \in \Omega$.

Proof. By applying Fourier transform to $\partial^n f / \partial v^n$ we have for all x in Ω

$$\sup_{y \in \mathbb{R}^N} \frac{\left| \frac{\partial^n f(x)}{\partial v^n} - \frac{\partial^n f(y)}{\partial v^n} \right|}{|y - x|^\kappa} \leq c \int_{\mathbb{R}^N} |\xi|^\gamma |\widehat{f}(\xi)| d\xi$$

and consequently

$$\left| \frac{\partial^n f(x)}{\partial v^n} \right| \leq c d_x^\kappa \int_{\mathbb{R}^N} |\xi|^\gamma |\widehat{f}(\xi)| d\xi$$

hence for a positive μ

$$\left| \frac{\partial^n f(x)}{\partial v^n} \right|^2 \leq c d_x^{2\kappa} \left(\int_{\mathbb{R}^N} (\mu + |\xi|^2)^{(\gamma-m)/2} (\mu + |\xi|^2)^{m/2} |\widehat{f}(\xi)| d^N \xi \right)^2.$$

It then follows from Cauchy–Schwartz that

$$\begin{aligned} \left| \frac{\partial^n f(x)}{\partial v^n} \right|^2 &\leq c d_x^{2\kappa} \left(\int_{\mathbb{R}^N} (\mu + |\xi|^2)^m |\widehat{f}(\xi)|^2 d^N \xi \right) \left(\int_{\mathbb{R}^N} \frac{1}{(\mu + |\xi|^2)^{m-\gamma}} d^N \xi \right) \\ &\leq \frac{c}{\varepsilon} d_x^{2\kappa} (\mu^{m(1-\varepsilon)} \|f\|_2^2 + \mu^{-m\varepsilon} Q(f)). \end{aligned}$$

Optimizing over μ to find the following that completes the proof:

$$\mu^m = \frac{\varepsilon}{1-\varepsilon} \frac{Q(f)}{\|f\|_2^2}. \quad \blacksquare$$

We proceed to find an upper bound for the heat kernel by applying Lemma 3.1 to $f_t := e^{-Ht}f$ but first we need a more comprehensive upper bound for $|\partial^n f_t(x)/\partial v^n|$ by applying the Spectral Theorem.

LEMMA 3.2. *If f_t is $e^{-Ht}f$ for some f in $L^2(\Omega)$ then*

$$(3.2) \quad Q(f_t) \leq \tilde{g}(t) \|f\|_2^2.$$

Proof. The inequality follows from

$$Q(f_t) \leq \|He^{-Ht}\| \|e^{-Ht}\| \|f\|_2^2$$

and an application of the Spectral Theorem. \blacksquare

We can now combine Lemmas 3.1 and 3.2 to yield our upper bound for the heat kernel.

LEMMA 3.3. *The heat kernel $k(t, x, y)$ generated by the differential operator H satisfies the inequalities:*

$$|k(t, x, y)| \leq c \left(1 - \frac{N+2\gamma}{2m}\right)^{-1} t^{-(N+2\gamma)/2m} d_x^\gamma d_y^\gamma \quad \text{when } t < \frac{2}{s},$$

$$|k(t, x, y)| \leq c \left(1 - \frac{N+2\gamma}{2m}\right)^{-1} e^{-st} d_x^\gamma d_y^\gamma \quad \text{when } t \geq \frac{2}{s}.$$

Proof. If $f_t := e^{-Ht}f$ then from Lemma 3.1 we have

$$\left| \frac{\partial^n f_t(x)}{\partial v^n} \right| \leq \frac{c}{\sqrt{\varepsilon}} d_x^\kappa Q(f_t)^{(1-\varepsilon)/2} \|f_t\|_2^\varepsilon.$$

Choosing v appropriately and integrating yields

$$\begin{aligned} \left| \int_{\Omega} k(t, x, u) f(u) d^N u \right| &\leq \frac{c}{\sqrt{\varepsilon}} d_x^\gamma \tilde{g}(t)^{(1-\varepsilon)/2} \|f\|_2^{1-\varepsilon} \|f_t\|_2^\varepsilon \\ &\leq \frac{c}{\sqrt{\varepsilon}} d_x^\gamma \tilde{g}(t)^{(1-\varepsilon)/2} e^{-ste} \|f\|_2. \end{aligned}$$

This inequality gives us a bound for the L_2 norm of $k(t, y, \cdot)$

$$\|k(t, y, \cdot)\|_2 \leq \frac{c}{\sqrt{\varepsilon}} d_x^\gamma \tilde{g}(t)^{(1-\varepsilon)/2} e^{-ste}$$

which can then be applied to obtain the required bounds:

$$\begin{aligned} |k(t, x, y)| &= \left| \int_{\Omega} k\left(\frac{t}{2}, x, u\right) k\left(\frac{t}{2}, u, y\right) d^N u \right| \leq \|k\left(\frac{t}{2}, x, \cdot\right)\|_2 \|k\left(\frac{t}{2}, y, \cdot\right)\|_2 \\ &\leq \frac{c}{\varepsilon} d_x^\gamma d_y^\gamma \tilde{g}\left(\frac{t}{2}\right)^{1-\varepsilon} e^{-ste}. \quad \blacksquare \end{aligned}$$

4. GAUSSIAN BOUNDS

Gaussian bounds exhibiting boundary decay can be given by interpolation between the bounds found in Lemma 3.3 and those obtained in Davies [4]. The drawback of this method however, is that the presence of the term c_3t does not imply the long-time exponential decay that we expect and would like to show. Dirichlet boundary conditions imply a positive spectral gap and hence exponential time *decay*. We give bounds that more concisely exhibit this behaviour.

One of the key features of hypothesis (2.3) is that many required operator inequalities can be reduced to proving the corresponding inequalities for polynomial symbols by applying Fourier transforms.

Barbatis and Davies [2] make a stronger assumption on the operator coefficients. They assume that for a strictly positive q

$$(4.1) \quad q^{-1} \sum_{|\alpha|=m, |\beta|=m} a_{0,\alpha\beta} \zeta_\alpha \bar{\zeta}_\beta \leq \sum_{|\alpha|=m, |\beta|=m} a_{\alpha\beta}(x) \zeta_\alpha \bar{\zeta}_\beta \leq q \sum_{|\alpha|=m, |\beta|=m} a_{0,\alpha\beta} \zeta_\alpha \bar{\zeta}_\beta$$

almost everywhere in Ω and the non-negative coefficient matrix $\mathbf{A}_0 = \mathbf{a}_{0,\alpha\beta}$ satisfies

$$(4.2) \quad \langle (-\Delta)^m f, g \rangle = \int_{\Omega} a_{0,\alpha\beta} D^\alpha f \overline{D^\beta g} d^N x$$

for all functions $f, g \in C_c^\infty(\Omega)$. They obtained the necessary estimates for the polyharmonic operator by way of Fourier transforms and an application of the polarization identity on the co-efficient matrix. We do not make this assumption here.

5. TWISTED QUADRATIC FORM INEQUALITY

Given x_0 in Ω and a unit vector \mathbf{a} in \mathbb{R}^N , we define the bounded function $\psi_{x_0, \mathbf{a}}$ on Ω

$$(5.1) \quad \psi_{x_0, \mathbf{a}}(x) := \langle x - x_0, \mathbf{a} \rangle.$$

Moreover given a real number λ and dropping the subscripts on $\psi_{x_0, \mathbf{a}}$ we define the multiplicative operator $e^{\lambda\psi}$

$$\begin{aligned} e^{\lambda\psi} : L^2(\Omega) &\rightarrow L^2(\Omega), \\ (e^{\lambda\psi} f)(x) &:= e^{\lambda\psi(x)} f(x) \end{aligned}$$

$e^{\lambda\psi}$ is a homeomorphism on $L^2(\Omega)$. The twisted operator $H_{\lambda\psi}$ is then defined as follows:

$$H_{\lambda\psi} f := e^{-\lambda\psi} H e^{\lambda\psi} f$$

with

$$\text{Dom}(H_{\lambda\psi}) = \{e^{-\lambda\psi} f : f \in \text{Dom}(H)\}.$$

More importantly we define the twisted quadratic form, $Q_{\lambda\psi}$ as follows:

$$\begin{aligned} Q_{\lambda\psi}(f) &:= Q(e^{\lambda\psi}f, e^{-\lambda\psi}f) \\ &= \sum_{\alpha, \beta} \int_{\Omega} a_{\alpha, \beta}(x) (D^{\alpha}(e^{\lambda\psi}f))(D^{\beta}(e^{-\lambda\psi}\bar{f})) d^N x \\ &= \sum_{\alpha, \beta} \int_{\Omega} a_{\alpha, \beta}(x) (e^{-\lambda\psi} D^{\alpha}(e^{\lambda\psi}f))(e^{\lambda\psi} D^{\beta}(e^{-\lambda\psi}\bar{f})) d^N x. \end{aligned}$$

By Leibniz, for each $f \in C_c^{\infty}(\Omega)$ we can expand

$$(5.2) \quad e^{-\lambda\psi} D^{\alpha} e^{\lambda\psi} f = \sum_{r \in V_{\alpha}} \binom{\alpha}{r} \lambda^{|\alpha-r|} a^{\alpha-r} D^r f.$$

It is then possible to show that the difference $\text{per}(\lambda) := Q_{\lambda\psi}(f) - Q(f)$ is

$$\sum_{\alpha, \beta} \int_{\Omega} a_{\alpha, \beta}(x) \sum' \binom{\alpha}{r} \binom{\beta}{s} \lambda^{|\alpha+\beta-(r+s)|} a^{\alpha-r} a^{\beta-s} D^r f D^s \bar{f}$$

where the summation \sum' runs over all r in V_{α} and s in V_{β} but where either $|r| < |\alpha|$ or $|s| < |\beta|$. The terms where both $r = \alpha$ and $s = \beta$ are incorporated in $Q(f)$. Since the coefficients of the operator are uniformly bounded we have for $c > 0$

$$|\text{per}(\lambda)| \leq c \sum_{\alpha, \beta} \sum' |\lambda|^{|\alpha+\beta-(r+s)|} \int_{\Omega} |D^r f| |D^s f| d^N x$$

and applying Cauchy–Schwartz

$$|\text{per}(\lambda)| \leq \sum_{1 \leq |\alpha| = |\beta| \leq m} \sum' \|\lambda^{|\alpha|-|r|} D^r f\|_2 \|\lambda^{|\beta|-|s|} D^s f\|_2.$$

From Lemma A.4 we see that for $\varepsilon < 1$

$$\begin{aligned} |\text{per}(\lambda)| &\leq c \sum_{1 \leq p \leq m} \sum' \|\lambda^{p-|r|} (-\Delta)^{|r|/2} f\|_2 \|\lambda^{p-|s|} (-\Delta)^{|s|/2} f\|_2 \\ &\leq c \sum_{1 \leq p \leq m} \varepsilon \|(-\Delta)^{p/2} f\|_2^2 + \varepsilon^{1-2p} \lambda^{2p} \|f\|_2^2. \end{aligned}$$

It follows from Lemma A.5 with $\rho = \varepsilon^{1-2m}$

$$|\text{per}(\lambda)| \leq c_1 \varepsilon (1 + \theta) Q(f) + c_1 \varepsilon^{1-2m} (1 + \theta s \varepsilon^{2m-1})^{2m} \lambda^{2m} \|f\|_2^2$$

and simplifying

$$|\text{per}(\lambda)| \leq c_1 \varepsilon (1 + \theta) Q(f) + c_1 \varepsilon^{1-2m} ([1 + \theta s] \lambda)^{2m} \|f\|_2^2.$$

Using

$$\text{Re}[Q(f) - Q_{\lambda\psi}(f)] = Q(f) - \text{Re}[Q_{\lambda\psi}(f)] \leq |Q(f) - Q_{\lambda\psi}(f)|$$

we have

$$(5.3) \quad [1 - c_1 \varepsilon (1 + \theta)] Q(f) \leq \text{Re} Q_{\lambda\psi}(f) + c_1 \varepsilon^{1-2m} ([1 + \theta s] \lambda)^{2m} \|f\|_2^2.$$

Moreover

$$(5.4) \quad |\operatorname{Im} Q_{\lambda\psi}(f)| \leq c_1 \varepsilon (1 + \theta) Q(f) + c_1 \varepsilon^{1-2m} ([1 + \theta s] \lambda)^{2m} \|f\|_2^2.$$

We note from Lemma A.5 that these inequalities are true for all positive θ .

6. SPECTRAL GAP

From the outset we know that H has a positive definite least eigenvalue s . We define

$$\widehat{H} := H - s$$

similarly

$$(6.1) \quad \widehat{H}_{\lambda\psi} f := e^{-\lambda\psi} H e^{\lambda\psi} f$$

and crucially

$$\widehat{Q}_{\lambda\psi}(f) := Q_{\lambda\psi}(f) - s \|f\|_2^2.$$

It is easy to see that the real and imaginary parts of the newly defined twisted form, $\widehat{Q}_{\lambda\psi}$ satisfy

$$(6.2) \quad [1 - c_1 \varepsilon (1 + \theta)] \widehat{Q}(f) \leq \operatorname{Re} \widehat{Q}_{\lambda\psi}(f) + c_1 \varepsilon^{1-2m} ([1 + \theta s] \lambda)^{2m} \|f\|_2^2$$

and

$$(6.3) \quad |\operatorname{Im} \widehat{Q}_{\lambda\psi}(f)| \leq c_1 \varepsilon (1 + \theta) \widehat{Q}(f) + c_1 \varepsilon^{1-2m} ([1 + \theta s] \lambda)^{2m} \|f\|_2^2.$$

7. TWISTED SEMIGROUP INEQUALITIES

LEMMA 7.1. *There is a constant $k > 0$ such that for all $c \geq k$ and all $0 < p < 1$*

$$Q'_{\lambda,\psi}(f) := \widehat{Q}_{\lambda\psi}(f) + c(1+p)(1+s)^{2m} \lambda^{2m} \|f\|_2^2$$

is a sectorial form with vertex at 0 and a semi-angle smaller than $\pi/2$. Moreover

$$\frac{p}{1+p} \widehat{Q}(f) \leq \operatorname{Re} \widehat{Q}_{\lambda\psi}(f) + c(1+p)(1+s)^{2m} \lambda^{2m} \|f\|_2^2.$$

Proof. With $\theta = (2 - (1+p))/(1+p)$ and $\varepsilon = 1/2c_1$ the second part of the RHS of (6.3)

$$c_1 \varepsilon^{1-2m} ([1 + \theta s] \lambda)^{2m} \|f\|_2^2$$

is less than

$$c_1^{2m} 2^{2m-1} (1+s)^{2m} \lambda^{2m} \|f\|_2^2$$

hence

$$\begin{aligned}
p|\operatorname{Im}Q'_{\lambda,\psi}(f)| &\leq \frac{p}{1+p}\widehat{Q}(f) + pc_1^{2m}2^{2m-1}(1+s)^{2m}\lambda^{2m}\|f\|_2^2 \\
&= [1 - c_1\varepsilon(1+\theta)]\widehat{Q}f + pc_1^{2m}2^{2m-1}(1+s)^{2m}\lambda^{2m}\|f\|_2^2 \\
&\leq \operatorname{Re}\widehat{Q}_{\lambda,\psi}(f) + (1+p)(c_1^{2m}2^{2m-1}(1+s)^{2m}\lambda^{2m})\|f\|_2^2 \\
&= \operatorname{Re}\widehat{Q}_{\lambda,\psi}(f) + c_2(1+p)(1+s)^{2m}\lambda^{2m}\|f\|_2^2 \\
&= \operatorname{Re}Q'_{\lambda,\psi}(f).
\end{aligned}$$

This then implies that

$$\frac{|\operatorname{Im}Q'_{\lambda,\psi}f|}{\operatorname{Re}Q'_{\lambda,\psi}f} \leq \frac{1}{p}$$

and consequently

$$|\operatorname{Arg} Q'_{\lambda,\psi}(f)| \leq \tan^{-1}\left(\frac{1}{p}\right) < \frac{\pi}{2}. \quad \blacksquare$$

We define the operator $H'_{\lambda,\psi}$

$$H'_{\lambda,\psi} := \widehat{H}_{\lambda,\psi} + c(1+s)^{2m}\lambda^{2m}$$

where $c > 0$ is such that

$$|\operatorname{Arg}\langle H'_{\lambda,\psi}f, f \rangle| < \frac{\pi}{2}.$$

We recall the following corollary from Kato [5].

COROLLARY 7.2. *Let β be angle such that $\pi/4 < \beta < \pi/2$ and set*

$$p = \frac{1}{\tan \beta}$$

Then $e^{-H'_{\lambda,\psi}z}$ is an analytic semigroup in the sector

$$S_\beta = \{z : |\operatorname{Arg}(z)| < \beta\};$$

moreover

$$\|e^{-H'_{\lambda,\psi}z}\| \leq 1.$$

For the proof see p. 492 of [5].

From Theorem 2.38 of [3] it is evident that there is a positive constant c_p such that

$$(7.1) \quad \|H'_{\lambda,\psi}e^{-H'_{\lambda,\psi}z}\| \leq \frac{c_p}{\operatorname{Re}z}$$

for all $z \in S_\beta$.

In the following estimates we let $\widehat{H}_{\lambda,\psi}$ be defined by (6.1).

LEMMA 7.3. *There is a positive constant c such that*

$$(7.2) \quad \|e^{-\widehat{H}_{\lambda,\psi}t}\| \leq \exp[c(1+s)^{2m}\lambda^{2m}t].$$

Proof. Let $f \in L^2(\Omega)$ and define $f_t := e^{-\widehat{H}_{\lambda\psi}t} f$, then solving

$$\begin{aligned} \frac{d}{dt} \|f_t\|_2^2 &= \langle -\widehat{H}_{\lambda\psi} f_t, f_t \rangle + \langle f_t, -\widehat{H}_{\lambda\psi} f_t \rangle = -2\operatorname{Re} \widehat{Q}_{\lambda\psi}(f_t) \\ &\leq 2c(1+s)^{2m} \lambda^{2m} \|f_t\|_2^2 \end{aligned}$$

proves the claim. ■

LEMMA 7.4. *Whenever $\beta \geq 0$, there is a positive constant c_2 such for any $0 < \alpha < 1$ we have*

$$(7.3) \quad \|\widehat{H}_{\lambda\psi} e^{-\widehat{H}_{\lambda\psi}t}\| + \beta(1+s)^{2m} \lambda^{2m} \|e^{-\widehat{H}_{\lambda\psi}t}\| \leq \frac{c_2}{\alpha t} e^{c(1+\alpha)(1+s)^{2m} \lambda^{2m} t}.$$

Proof. Applying the triangle inequality gives us

$$\|\widehat{H}_{\lambda\psi} e^{-\widehat{H}_{\lambda\psi}t}\| e^{-c(1+s)^{2m} \lambda^{2m} t} \leq \|H'_{\lambda,\psi} e^{-H'_{\lambda,\psi}t}\| + c(1+s)^{2m} \lambda^{2m} \|e^{-H'_{\lambda,\psi}t}\|$$

and it follows from (7.1) and Lemma 7.3

$$\|\widehat{H}_{\lambda\psi} e^{-\widehat{H}_{\lambda\psi}t}\| \leq \frac{c_1}{t} e^{c(1+s)^{2m} \lambda^{2m} t} + c(1+s)^{2m} \lambda^{2m} e^{c(1+s)^{2m} \lambda^{2m} t}.$$

Then the LHS of (7.3) is bounded above by

$$(7.4) \quad \frac{c_1}{t} e^{c(1+s)^{2m} \lambda^{2m} t} + c(1+\beta)(1+s)^{2m} \lambda^{2m} e^{c(1+s)^{2m} \lambda^{2m} t}.$$

For positive real x we can re-write $x e^{xt}$ as

$$\frac{1}{\alpha} e^{(1+\alpha)xt} \cdot x \alpha e^{-\alpha xt}$$

for some $\alpha > 0$. We can then observe that

$$x e^{xt} \leq \frac{e^{(1+\alpha)xt}}{\alpha} \cdot \frac{e^{-1}}{t}$$

and see that similarly

$$c(1+s)^{2m} \lambda^{2m} e^{c(1+s)^{2m} \lambda^{2m} t} \leq \frac{e^{-1}}{\alpha t} e^{(1+\alpha)c(1+s)^{2m} \lambda^{2m} t}.$$

Substitution into (7.4) attains the claimed inequality. ■

LEMMA 7.5. *Let $f \in L^2(\Omega)$ and define $\widehat{f}_t := e^{-\widehat{H}_{\lambda\psi}t} f$ then there are positive constants c_1 and c_2 such that*

$$(7.5) \quad \widehat{Q}(\widehat{f}_t) \leq \frac{c_1}{\alpha t} e^{c_2(1+s)^{2m} \lambda^{2m} t} \|f\|_2^2.$$

Proof. From Lemma 7.1 we have that for some positive constants c_1 and c_2

$$\begin{aligned} \widehat{Q}(\widehat{f}_t) &\leq c_1 \operatorname{Re} \widehat{Q}_{\lambda\psi}(\widehat{f}_t) + c_2(1+s)^{2m} \lambda^{2m} \|\widehat{f}_t\|_2^2 \\ &\leq c_1 \|\widehat{H}_{\lambda\psi} \widehat{f}_t\|_2 \|\widehat{f}_t\|_2 + c_2(1+s)^{2m} \lambda^{2m} \|\widehat{f}_t\|_2^2. \end{aligned}$$

By using Lemma 7.4 we can see that for $0 < \alpha < 1$

$$\begin{aligned}\widehat{Q}(\widehat{f}_t) &\leq \frac{c_1}{\alpha t} e^{c(1+\alpha)(1+s)^{2m}\lambda^{2m}t} \|f\|_2 \|\widehat{f}_t\|_2 \\ &\leq \frac{c_1}{\alpha t} e^{2c(1+\alpha)(1+s)^{2m}\lambda^{2m}t} \|f\|_2^2. \quad \blacksquare\end{aligned}$$

COROLLARY 7.6. *There are positive constants c_1 and c_2 such that*

$$Q(e^{-H_{\lambda\psi}t} f) \leq \frac{c_1}{\alpha t} e^{c_2(1+s)^{2m}\lambda^{2m}t - 2st} \|f\|_2^2.$$

Proof. By substitution from

$$\widehat{Q}(\widehat{f}_t) = Q(\widehat{f}_t) - s\|\widehat{f}_t\|_2^2 \quad \text{and} \quad \widehat{f}_t = e^{-\widehat{H}_{\lambda\psi}t} f = e^{-H_{\lambda\psi}t} e^{-st} f$$

it can be seen that

$$\widehat{Q}(\widehat{f}_t) = e^{2st} Q(e^{-H_{\lambda\psi}t} f) - s\|\widehat{f}_t\|_2^2,$$

hence for $0 < \alpha < 1$

$$Q(e^{-H_{\lambda\psi}t} f) \leq e^{-2st} [\widehat{Q}(\widehat{f}_t) + s\|\widehat{f}_t\|_2^2] \leq e^{-2st} \left[\frac{c_1}{\alpha t} e^{c_2(1+s)^{2m}\lambda^{2m}t} \|f\|_2^2 + s\|\widehat{f}_t\|_2^2 \right].$$

Applying the estimate from Lemma 7.3 completes the proof. \blacksquare

8. HEAT KERNEL BOUNDS

THEOREM 8.1. *The integral kernel $k_{\lambda,\psi}(t, x, y)$ of $e^{-H_{\lambda\psi}t}$ satisfies the inequality*

$$(8.1) \quad k|k_{\lambda,\psi}(t, x, y)| \leq \frac{c}{\varepsilon t^{1-\varepsilon}} d_x^\gamma d_y^\gamma e^{[c_2(1+s)^{2m}\lambda^{2m} - s]t}$$

for some positive constants c and c_2 .

Proof. For $f \in L^2(\Omega)$ we define $f_t := e^{-H_{\lambda\psi}t} f$. From Lemma 3.1

$$\left| \frac{\partial^n f_t(x)}{\partial \mathbf{v}^n} \right| \leq \frac{c}{\sqrt{\varepsilon}} d_x^K Q(f_t)^{(1-\varepsilon)/2} \|f_t\|_2^\varepsilon$$

and from Corollary 7.6

$$(8.2) \quad \left| \frac{\partial^n f_t(x)}{\partial \mathbf{v}^n} \right| \leq \frac{c}{t^{(1-\varepsilon)/2} \sqrt{\varepsilon}} d_x^K e^{((1-\varepsilon)/2)[c_2(1+s)^{2m}\lambda^{2m} - 2s]t} \|f\|_2^{1-\varepsilon} \|f_t\|_2^\varepsilon.$$

Recalling that $f_t = e^{-H_{\lambda\psi}t} f = e^{-st} e^{-\widehat{H}_{\lambda\psi}t} f$ then with Lemma 7.3 we have the estimate

$$\|f_t\|_2^\varepsilon \leq \exp(\varepsilon c_2(1+s)^{2m}\lambda^{2m}t) e^{-\varepsilon st} \|f\|_2^\varepsilon.$$

Substituting this estimate into (8.2)

$$\left| \frac{\partial^n f_t(x)}{\partial \mathbf{v}^n} \right| \leq \frac{c}{t^{(1-\varepsilon)/2} \sqrt{\varepsilon}} d_x^K e^{[c_2(1+s)^{2m}\lambda^{2m} - s]t} \|f\|_2.$$

Integrating along the path to the boundary

$$\left| \int_{\Omega} k_{\lambda, \psi}(t, x, u) f(u) \, d^N u \right| \leq \frac{c}{t^{(1-\varepsilon)/2} \sqrt{\varepsilon}} d_x^\gamma e^{[c_2(1+s)^{2m} \lambda^{2m} - s]t} \|f\|_2.$$

Following a similar argument to that in the proof to Lemma 3.3

$$|k_{\lambda, \psi}(t, x, y)| \leq \|k_{\lambda, \psi}(\frac{t}{2}, x, \cdot)\|_2 \|k_{\lambda, \psi}(\frac{t}{2}, y, \cdot)\|_2$$

to yield the upper bound

$$|k_{\lambda, \psi}(t, x, y)| \leq \frac{c}{\varepsilon t^{1-\varepsilon}} d_x^\gamma d_y^\gamma e^{[c_2(1+s)^{2m} \lambda^{2m} - s]t}. \quad \blacksquare$$

THEOREM 8.2. *The integral kernel $k(t, x, y)$ of e^{-Ht} satisfies the inequality*

$$|k(t, x, y)| \leq c_1 \left(1 - \frac{N+2\gamma}{2m}\right)^{-1} t^{-(N+2\gamma)/2m} d_x^\gamma d_y^\gamma \exp\left(-c_2 \frac{|x-y|^{2m/(2m-1)}}{t^{1/(2m-1)}} - st\right)$$

for some positive constants c_1 and c_2 and where s is the least eigenvalue and $0 \leq \gamma < m - N/2$

Proof. We demonstrate the proof in two stages. Firstly optimising over ψ and then optimising over λ .

From Lemma B.4 we know that

$$k(t, x, y) = e^{-\lambda\psi(x)} k_{\lambda, \psi}(t, x, y) e^{\lambda\psi(y)}$$

recalling the definition of ψ from (5.1), for some unit vector \mathbf{a}

$$\psi(\mathbf{y}) - \psi(\mathbf{x}) = \langle \mathbf{y} - \mathbf{x}, \mathbf{a} \rangle.$$

If \mathbf{a} is such that

$$\psi(\mathbf{y}) - \psi(\mathbf{x}) = -|\mathbf{y} - \mathbf{x}|$$

then substitution into the estimate (8.1) yields

$$(8.3) \quad |k(t, x, y)| \leq \frac{c}{\varepsilon t^{1-\varepsilon}} d_x^\gamma d_y^\gamma e^{[c_2(1+s)^{2m} \lambda^{2m} - s]t - \lambda|x-y|}.$$

Optimising the exponent of the RHS over λ we find

$$\lambda^{2m-1} = \frac{|x-y|}{2mc_2(1+s)^{2m}t}.$$

Substituting back into (8.3) we find there is a positive constant c_2

$$(8.4) \quad |k(t, x, y)| \leq \frac{c}{\varepsilon t^{1-\varepsilon}} d_x^\gamma d_y^\gamma \exp\left(-c_2 \frac{|x-y|^{2m/(2m-1)}}{((1+s)^{2m}t)^{1/(2m-1)}} - st\right).$$

Recalling that $\varepsilon = 1 - (N + 2\gamma)/2m$ we have the required estimate. \blacksquare

Appendix A. POLYNOMIAL AND OPERATOR SYMBOL INEQUALITIES

When perturbing our quadratic form Q , the resulting twisted form $Q_{\lambda,\psi}$ generates cross terms of the form $\lambda^p D^\alpha$. We can use ellipticity and Fourier transform to estimate these terms with the polyharmonic $(-\Delta)^{m/2}$ for $m > p + |\alpha|$

$$\begin{aligned} \|\lambda^p D^\alpha f\|_2^2 &\leq \int_{\mathbb{R}^N} (c_1 |\xi|^{p+|\alpha|} + c_2 |\lambda|^{p+|\alpha|}) |\widehat{f}(\xi)|^2 d^N \xi \\ &\leq c_1 (\|(-\Delta)^{m/2} f\|_2^2 + 1) + c_2 (1 + \lambda^{2m} \|f\|_2^2). \end{aligned}$$

However a more detailed decomposition of these polynomials is required to attain tighter bounds on $\|\lambda^p D^\alpha f\|_2^2$. So that we can show exponential decay of the heat kernel in long time asymptotics.

LEMMA A.1. *If a, b, p and q are all positive constants then*

$$a^p b^q \leq \varepsilon a^{p+q} + c_{p,q} \varepsilon^{-p/q} b^{p+q}$$

for all $\varepsilon > 0$ where $c_{p,q} := (p/(p+q))^{p/q} - (p/(p+q))^{1+p/q}$ is strictly positive and strictly less than 1.

The proof follows from maximising $x^p - \varepsilon x^{p+q}$ and substituting $x = a/b$.

LEMMA A.2. *Given $p > q > 0$ there is a strictly positive constant $c_{q,p}$ such that for all $f \in C_c^\infty(\Omega)$*

$$\|(-\Delta)^q f\|_2 < c_{q,p} \|(-\Delta)^p f\|_2.$$

The proof follows from the Spectral Theorem.

LEMMA A.3. *If $f \in C_c^\infty(\Omega)$, $\lambda \in \mathbb{R}$ and p is a positive integer then whenever r is a multi-index for which $|r| < p$*

$$\|\lambda^{p-|r|} D^r f\|_2 \leq \varepsilon \|(-\Delta)^{p/2} f\|_2 + \varepsilon^{-|r|/(p-|r|)} |\lambda|^p \|f\|_2$$

for any $\varepsilon > 0$.

Proof. From the isometry of the Fourier transform we see that

$$\|\lambda^{p-|r|} D^r f\|_2^2 = \int_{\Omega} \lambda^{2(p-|r|)} |D^r f|^2 d^N x = \int_{\mathbb{R}^N} \lambda^{2(p-|r|)} |(i\xi)^r|^2 |\widehat{f}(\xi)|^2 d^N \xi$$

then using $|(i\xi)^r|^2 \leq |\xi|^{2|r|}$ and Lemma A.1. it follows that

$$\begin{aligned} \|\lambda^{p-|r|} D^r f\|_2^2 &\leq \int_{\mathbb{R}^N} [\varepsilon |\xi|^{2p} + \varepsilon^{-|r|/(p-|r|)} |\lambda|^{2p}] |\widehat{f}(\xi)|^2 d^N \xi \\ &\leq \varepsilon \|(-\Delta)^{p/2} f\|_2^2 + \varepsilon^{-|r|/(p-|r|)} |\lambda|^{2p} \|f\|_2^2. \end{aligned}$$

Rescaling ε recovers the required inequality. ■

LEMMA A.4. *If \mathbf{r} and \mathbf{s} are two multi-indices such that $|\mathbf{s}| \leq p - 1$ and $|\mathbf{r}| \leq p$ where p is a positive integer and $\lambda \in \mathbb{R}$ then*

$$\|\lambda^{p-|\mathbf{r}|}(-\Delta)^{|\mathbf{r}|/2}f\|_2 \|\lambda^{p-|\mathbf{s}|}(-\Delta)^{|\mathbf{s}|/2}f\|_2 \leq \varepsilon \|(-\Delta)^{p/2}f\|_2^2 + 2^{2p-1}\varepsilon^{1-2p}\lambda^{2p}\|f\|_2^2$$

for all $\varepsilon < 2$.

Proof. Case $|\mathbf{r}| = p$.

We apply Lemma A.3:

$$\begin{aligned} \|\lambda^{p-|\mathbf{r}|}(-\Delta)^{|\mathbf{r}|/2}f\|_2 \|\lambda^{p-|\mathbf{s}|}(-\Delta)^{|\mathbf{s}|/2}f\|_2 \\ \leq \|(-\Delta)^{p/2}f\|_2 (\varepsilon \|(-\Delta)^{p/2}f\|_2 + \varepsilon^{-|\mathbf{s}|/(p-|\mathbf{s}|)}|\lambda|^p\|f\|_2) \\ = \varepsilon \|(-\Delta)^{p/2}f\|_2^2 + (\varepsilon^{-|\mathbf{s}|/(p-|\mathbf{s}|)}|\lambda|^p\|f\|_2) \|(-\Delta)^{p/2}f\|_2. \end{aligned}$$

Using the estimate $|ab| < (1/\varepsilon)a^2 + \varepsilon b^2$ we show that the above is

$$\begin{aligned} &\leq \varepsilon \|(-\Delta)^{p/2}f\|_2^2 + \frac{1}{\varepsilon} \cdot \varepsilon^{-2|\mathbf{s}|/(p-|\mathbf{s}|)}|\lambda|^{2p}\|f\|_2^2 + \varepsilon \|(-\Delta)^{p/2}f\|_2^2 \\ &\leq 2\varepsilon \|(-\Delta)^{p/2}f\|_2^2 + \varepsilon^{-(p+|\mathbf{s}|)/(p-|\mathbf{s}|)}|\lambda|^{2p}\|f\|_2^2. \end{aligned}$$

Imposing the condition $\varepsilon < 1$ and maximizing $\varepsilon^{-(p+|\mathbf{s}|)/(p-|\mathbf{s}|)}$ over \mathbf{s} we have the inequality

$$\|\lambda^{p-|\mathbf{r}|}(-\Delta)^{|\mathbf{r}|/2}f\|_2 \|\lambda^{p-|\mathbf{s}|}(-\Delta)^{|\mathbf{s}|/2}f\|_2 \leq 2\varepsilon \|(-\Delta)^{p/2}f\|_2^2 + \varepsilon^{1-2p}|\lambda|^{2p}\|f\|_2^2.$$

The proof for this case is completed on rescaling ε .

Case $|\mathbf{r}| < p$ follows from Lemma A.3. ■

Having completed this decomposition, we obtain an estimate for lower order operators in terms of the higher order operator.

LEMMA A.5. *There is a positive constant c_1 such for all $\rho > 0$, $\theta > 0$ and positive integer $p \leq m$*

$$\|(-\Delta)^{p/2}f\|_2^2 + \rho\lambda^{2p}\|f\|_2^2 \leq c_1(1 + \theta)Q(f) + c_1\rho\left(1 + \frac{\theta s}{\rho}\right)^{2m}\lambda^{2m}\|f\|_2^2$$

for all $f \in C_c^\infty(\Omega)$ and with s equal to the bottom eigenvalue.

Proof. We can show applying Lemma A.1 that for each $\mu > 0$ this is

$$(A.1) \quad \|(-\Delta)^{p/2}f\|_2^2 + \rho\lambda^{2p}\|f\|_2^2 \leq \|(-\Delta)^{p/2}f\|_2^2 + \rho\mu\|f\|_2^2 + \rho\mu^{-(m-p)/p}\lambda^{2m}\|f\|_2^2.$$

Applying Lemma A.2 and ellipticity whilst recalling that we have positive-definite spectral gap s

$$\begin{aligned} &\|(-\Delta)^{p/2}f\|_2^2 + \rho\lambda^{2p}\|f\|_2^2 \\ &\leq c_1\|(-\Delta)^{m/2}f\|_2^2 + \rho m\mu\|f\|_2^2 + \rho m(1 + \mu)^{m-1}\lambda^{2m}\|f\|_2^2 \\ &\leq c_1(1 + \theta)Q(f) - c_1\theta s\|f\|_2^2 + \rho m\mu\|f\|_2^2 + \rho m(1 + \mu)^{m-1}\lambda^{2m}\|f\|_2^2 \end{aligned}$$

we can then set $\mu = c_1\theta s/m\rho$. ■

Appendix B. DAVIES' TWISTED OPERATORS AND THE CANONICAL FUNCTIONAL CALCULUS

The two definitions are consistent

$$Q_{\lambda\psi}(f) = \langle H^{1/2}e^{\lambda\psi}f, H^{1/2}e^{-\lambda\psi}f \rangle = \langle e^{-\lambda\psi}He^{\lambda\psi}f, f \rangle = \langle H_{\lambda\psi}f, f \rangle.$$

LEMMA B.1. *H and $H_{\lambda\psi}$ have the same spectrum.*

Proof. Given a sequence of functions f_n where $(H - z)f_n \rightarrow 0$ we have $(H_{\lambda\psi} - z)(e^{-\lambda\psi}f_n) \rightarrow 0$. ■

LEMMA B.2. *For each $f \in L^2(\Omega)$ and z in the resolvent set of H we have*

$$(z - H_{\lambda\psi})^{-1}f = e^{-\lambda\psi}(z - H)^{-1}e^{\lambda\psi}f.$$

Proof. Let $\mathbb{B} = (z - H_{\lambda\psi})^{-1}$ then

$$\mathbb{B}(z - H_{\lambda\psi})f = f$$

which is just

$$\mathbb{B}e^{-\lambda\psi}(z - H)e^{\lambda\psi}f = f$$

and out statement follows. ■

COROLLARY B.3. *For $f \in C_0(\mathbb{R})$ we have a canonical functional calculus for the twisted operator given by*

$$f(H_{\lambda\psi}) := e^{-\lambda\psi}f(H)e^{\lambda\psi}.$$

LEMMA B.4. *If $f \in C_0(\mathbb{R})$ and $k_f(x, y)$ is the integral kernel of the operator $f(H)$ then $f(H_{\lambda\psi})$ has integral kernel $k_{f, \lambda\psi}(x, y)$ where*

$$k_{f, \lambda\psi}(x, y) = e^{-\lambda\psi(x)}k_f(x, y)e^{\lambda\psi(y)}.$$

Proof. Let $v \in L^2(\Omega)$ then

$$\begin{aligned} \int_{\Omega} k_{f, \lambda\psi}(x, y) v(y) dy &= (f(H_{\lambda\psi})v)(x) = (e^{-\lambda\psi}f(H)e^{\lambda\psi}v)(x) \\ &= e^{-\lambda\psi(x)} \int_{\Omega} k_f(x, y) e^{\lambda\psi(y)} v(y) dy. \quad \blacksquare \end{aligned}$$

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