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SHARP CONSTANTS IN HIGHER-ORDER HEAT KERNEL BOUNDS

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We consider a space X of polynomial type and a self-adjoint operator on $L^2(X)$ which is assumed to have a heat kernel satisfying second-order Gaussian bounds. We prove that any power of the operator has a heat kernel satisfying Gaussian bounds with a precise constant in the Gaussian. This constant was previously identified by Barbatis and Davies in the case of powers of the Laplace operator on $\mathbf{R}^N$. In this case we prove slightly sharper bounds and show that the above-mentioned constant is optimal.

1. INTRODUCTION

In [**1**] Barbatis and Davies considered the problem of obtaining sharp constants in Gaussian heat kernel bounds for a class of higher order elliptic operators acting on $L^2\left(\mathbf{R}^N\right)$. In particular, they obtained the following result. Let $K_t^{(m)}$ denote the heat kernel for the operator $\Delta^{m/2}$, where $\Delta = -\sum_{j=1}^{N} \partial_j^2$ is the ordinary Laplacian on $\mathbf{R}^N$ and m is a positive even integer with $m > N$. Then for each $r > 1$ there exists $c_r > 0$, depending only on m, N, and r, such that

$$(1) \qquad \left|K_t^{(m)}(x\,;y)\right| \leqslant c_r\, t^{-N/m} e^{-(b_m/r)(d(x\,;y)^m/t)^{1/(m-1)}} \quad x, y \in \mathbf{R}^N,\ t > 0,$$

where the constant b_m is given by

$$(2) \qquad b_m = (m-1)\, m^{-m/(m-1)} \sin\left(\pi/(2m-2)\right)$$

and $d(x\,;y) = \left(\sum_{j=1}^{N} (x_j - y_j)^2\right)^{1/2}$ is the Euclidean distance.

In this paper, we improve this result in two directions. In Section 2, we prove Theorem 1, which may roughly be stated as follows. Let H be a nonnegative self-adjoint operator on $L^2(X;\mu)$ for a measure space (X,μ) with a metric d which satisfies a uniform condition of polynomial growth. If the heat kernel for H satisfies second-order

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Gaussian bounds with a factor which may be chosen arbitrarily close to $b_2 = 1/4$ in the exponential, then the heat kernel for $H^{m/2}$ satisfies m-th order Gaussian bounds with a factor arbitrarily close to b_m in the exponential. Thus the constant b_m is typical for powers of a general class of self-adjoint operators. This is not clear from the analysis of [**1**], which uses the Fourier theory of $L^2\left(\mathbf{R}^N\right)$.

The second-order Gaussian bounds with a factor arbitrarily close to $1/4$ are characteristic for a variety of second-order elliptic, or subelliptic, differential operators over manifolds. For example, second-order uniformly elliptic operators in divergence form with real measurable symmetric coefficients on $\mathbf{R}^N$, and left-invariant sublaplacians on Lie groups of polynomial growth, satisfy the assumptions of Theorem 1 [**3, 6, 8**].

Robinson and ter Elst showed in unpublished work that Gaussian bounds for powers of an operator may be deduced from second-order Gaussian bounds for the operator itself. A similar result, under different hypotheses, was proved by Saloff-Coste [**7**]. Robinson and ter Elst's proof used a Cauchy integral representation for the semigroup $S_t^{(m)} = e^{-tH^{m/2}}$ together with a partial fraction decomposition of the resolvent of $H^{m/2}$ in terms of the resolvent of H (a similar decomposition was previously used in [**5**]). Our proof of Theorem 1 follows their method, but in order to obtain the sharp constant b_m we need more precise bounds on the kernel of the resolvent (see Lemma 5 below) and more careful choices of certain parameters.

In Section 3 we return to the special case of the operator $\Delta^{m/2}$ on $\mathbf{R}^N$. Using Fourier theory we prove that (1) holds with $r = 1$, and for all m and N without the restriction $m > N$ of [**1**]. Finally we confirm the conjecture of [**1**] that the constant b_m is optimal, by showing that the bounds (1) cannot hold when $0 < r < 1$.

2. Powers of self-adjoint operators

Let (X, d) be a metric space and μ a positive measure on X. We assume that the ball $B(x;r) = \left\{ y \in X : d(x;y) < r \right\}$ is μ-measurable for each $x \in X$ and $r > 0$, and set $V(x;r) = \mu\left(B(x;r)\right)$. We further assume that the space has uniform polynomial growth, in the sense that there are integers $D' \geqslant 1$ and $D \geqslant 0$ such that

$$C^{-1} r^{D'} \leqslant V(x;r) \leqslant C\, r^{D'}, \quad 0 < r \leqslant 1,$$
$$C^{-1} r^{D} \leqslant V(x;r) \leqslant C\, r^{D}, \quad r \geqslant 1,$$

for some $C > 0$ and all x. (The integers D' and D are often called the dimensions at zero and infinity respectively.) Then μ is σ-finite, because $X = \bigcup_{n=1}^{\infty} B(x_0; n)$ is a countable union of balls. The volume growth of balls is measured by the function V defined by $V(r) = r^{D'}$ or $V(r) = r^D$ according as $0 < r < 1$ or $r \geqslant 1$.

Let H be a nonnegative self-adjoint operator on $L^2 = L^2(X;\mu)$. Then H generates a holomorphic semigroup $S_z = e^{-zH}$ on L^2, defined for all $z \in \mathbf{C}$ with $\operatorname{Re} z > 0$. We assume that S_t has a continuous kernel $K_t : X \times X \to \mathbf{C}$ for each $t > 0$ which satisfies Gaussian bounds with a factor arbitrarily close to $1/4$ in the exponential. That is,

$$(S_t f)(x) = \int_X d\mu(y)\, K_t(x\,;y) f(y)\,, \quad f \in L^2\,,$$

and for each $r > 1$ there exists $c_r > 0$ such that

$$\left|K_t(x\,;y)\right| \leqslant c_r\, V(t)^{-1/2} e^{-d^2/(4rt)}$$

for all $t > 0$ and $x, y \in X$. Here, as elsewhere, we abbreviate $d(x\,;y)$ as d. Let m be a positive even integer. Then the operator $H^{m/2}$ is nonnegative self-adjoint on L^2 and generates a semigroup $S_t^{(m)} = e^{-tH^{m/2}}$ on L^2.

THEOREM 1. *Suppose that (X, d, μ), and H acting on $L^2(X;\mu)$, satisfy the above assumptions, and let $m \geqslant 4$ be an even integer. Then the semigroup $S_t^{(m)} = e^{-tH^{m/2}}$ has an integral kernel $K_t^{(m)}$. Moreover for each $r > 1$ there exists $c'_r > 0$, depending on (X, d, μ), H, m, and r, such that*

$$\left|K_t^{(m)}(x\,;y)\right| \leqslant c'_r\, V(t)^{-1/m} e^{-(b_m/r)\,(d^m/t)^{1/(m-1)}}\,, \qquad d = d(x\,;y)\,,$$

for all $t > 0$ and $x, y \in X$.

The first step in the proof of Theorem 1 is to derive uniform bounds.

LEMMA 2. *The semigroup $S_t^{(m)}$ has an integral kernel $K_t^{(m)}$ satisfying bounds*

$$\left|K_t^{(m)}(x\,;y)\right| \leqslant c\, V(t)^{-1/m}$$

for all $t > 0$ and $x, y \in X$.

PROOF: Let $\|\cdot\|_{p\to q}$ denote the norm of a bounded linear operator from $L^p(X;\mu)$ to $L^q(X;\mu)$. Then

$$\|S_t\|_{2\to\infty} \leqslant \sup_{x\in X} \left(\int d\mu(y) \left|K_t(x\,;y)\right|^2\right)^{1/2} \leqslant c\, V(t)^{-1/4}$$

where the second inequality follows from the Gaussian bounds on K by a quadrature argument (see for example [**4**, Proposition 2.1]). Fix $k > N/2$, where $N = D' \vee D$. For each $\rho > 0$ one has the identity

$$(I + \rho H)^{-k/2} = \Gamma(k/2)^{-1} \int_0^\infty dt\, e^{-t} t^{-1+(k/2)}\, S_{t\rho}$$

and using a volume inequality $V(t\rho)^{-1/4} \leqslant c\left(1 + t^{-N/4}\right) V(\rho)^{-1/4}$ one finds that

$$\left\|(I + \rho H)^{-k/2}\right\|_{2\to\infty} \leqslant c'\, V(\rho)^{-1/4} \int_0^\infty dt\, e^{-t} t^{1+(k/2)} \left(1 + t^{-N/4}\right) = c''\, V(\rho)^{-1/4}$$

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for all $\rho > 0$. Using this estimate and spectral theory gives

$$\left\|S_t^{(m)}\right\|_{2\to\infty} \leqslant \left\|\left(I+t^{2/m}H\right)^{-k/2}\right\|_{2\to\infty}\left\|\left(I+t^{2/m}H\right)^{k/2}S_t^{(m)}\right\|_{2\to 2} \leqslant c'\,V(t)^{-1/(2m)}\,.$$

Therefore

$$\left\|S_t^{(m)}\right\|_{1\to\infty} \leqslant \left(\left\|S_{t/2}^{(m)}\right\|_{2\to\infty}\right)^2 \leqslant c\,V(t)^{-1/m}$$

and the lemma follows by the Dunford–Pettis Theorem. ∎

To derive Gaussian bounds, following an unpublished argument of ter Elst and Robinson, we first reduce to the case where $D' = D \geqslant 4$.

Lemma 3. *If Theorem* 1 *holds when $D' = D \geqslant 4$, then it holds generally.*

Proof: Suppose that the quadruple (X, d, μ, H) satisfies the assumptions of Theorem 1. If $D' > D$ define $X_2 = G^{D'-D} \times \mathbf{R}^3$ where G is the three-dimensional Heisenberg group, if $D' < D$ define $X_2 = \mathbf{T}^{D-D'} \times \mathbf{R}^3$ and if $D' = D$ define $X_2 = \mathbf{R}^3$. Then X_2 is a Lie group and we let μ_2 be the (bi-invariant) Haar measure on X_2. Choose left-invariant vector fields $A_1, \ldots, A_k$ which form a vector space basis for the Lie algebra of X_2, and let d_2 be the left-invariant distance and $H_2 = -\sum_{j=1}^{k} A_j^2$ the Laplacian associated with this choice. Then (X_2, d_2, μ_2, H_2) satisfies the assumptions of Theorem 1; in particular, the kernel $K_{2,t}$ of e^{-tH_2} satisfies Gaussian bounds with a factor arbitrarily close to $1/4$ [**6, 8**]. If D_2' and D_2 are the dimensions at zero and infinity of (X_2, d_2, μ_2) then $D_2' + D' = D_2 + D \geqslant 4$. Moreover, since $H_2^{m/2}1 = 0$ it follows that $1 = \left(S_{2,t}^{(m)}1\right)(x_2) = \int_{X_2} d\mu_2(y_2)\, K_{2,t}^{(m)}(x_2\,; y_2)$ for all $x_2 \in X_2$, where $K_{2,t}^{(m)}$ is the kernel of $S_{2,t}^{(m)} = e^{-tH_2^{m/2}}$.

Now define $\widetilde{X} = X \times X_2$ and let $\tilde{d}\left((x, x_2)\,; (y, y_2)\right)^2 = d(x\,; y)^2 + d_2(x_2\,; y_2)^2$ for (x, x_2), $(y, y_2) \in \widetilde{X}$. Let $\tilde{\mu} = \mu \times \mu_2$ be the product measure on $\widetilde{X}$, and set $\widetilde{H} = H \otimes I + I \otimes H_2$, where we have identified $L^2\left(\widetilde{X}\right) = L^2(X) \otimes L^2(X_2)$. Then the quadruple $\left(\widetilde{X}, \tilde{d}, \tilde{\mu}, \widetilde{H}\right)$ satisfies the assumptions of Theorem 1, and moreover the dimensions at zero and infinity of $\left(\widetilde{X}, \tilde{d}, \tilde{\mu}\right)$ are equal and not less than 4. Thus by assumption, the kernel $\widetilde{K}_t^{(m)}$ of $\widetilde{S}_t^{(m)} = e^{-t\widetilde{H}^{m/2}}$ satisfies Gaussian bounds with a factor arbitrarily close to b_m. One easily sees that

$$\widetilde{K}_t^{(m)}\left((x, x_2)\,; (y, y_2)\right) = K_t^{(m)}(x\,; y)\, K_{2,t}^{(m)}(x_2\,; y_2)$$

for all $x, y \in X$ and $x_2, y_2 \in X_2$. Since $\int_{X_2} d\mu_2(y_2)\, K_{2,t}^{(m)}(x_2\,; y_2) = 1$ we obtain

$$K_t^{(m)}(x\,; y) = \int_{X_2} d\mu_2(y_2)\, \widetilde{K}_t^{(m)}\left((x, x_2)\,; (y, y_2)\right) \quad .$$

But for any $r > 1$ and $r' \in (1, r)$, the kernel $\widetilde{K}^{(m)}$ satisfies bounds

$$\begin{aligned}\left|\widetilde{K}_t^{(m)}\left((x, x_2)\,; (y, y_2)\right)\right| &\leqslant c_{r'}\, \widetilde{V}(t)^{-1/m}\, e^{-(b_m/r')\left(\tilde{d}^m/t\right)^{1/(m-1)}} \\ &\leqslant c_{r'}\, V(t)^{-1/m}\, e^{-(b_m/r)(d^m/t)^{1/(m-1)}}\, V_2(t)^{-1/m}\, e^{-\varepsilon\left(d_2^m/t\right)^{1/(m-1)}}\end{aligned}$$

where $\varepsilon = (b_m/r') - (b_m/r) > 0$. Integrating these bounds over X_2 with respect to y_2 yields Gaussian bounds on $K_t^{(m)}$ with a factor of b_m/r, as required. □

In the remainder of the proof of Theorem 1 we shall assume that $D' = D \geqslant 4$, so that $V(r) = r^D$ for all $r > 0$.

Lemma 4. *The operator $S_z = e^{-zH}$ has a kernel K_z satisfying bounds*

$$\left|K_z(x\,;y)\right| \leqslant c_r\,(\operatorname{Re} z)^{-D/2}\,e^{-\operatorname{Re}\{d^2/(4rz)\}} = c_r\,|z|^{-D/2}(\cos\theta)^{-D/2}e^{-\cos\theta\, d^2/(4r|z|)}$$

for all $z \in \mathbf{C}$ with $\operatorname{Re} z > 0$ and $\theta = \arg z$, all $r > 1$ and all $x, y \in X$.

Proof: The existence of the kernel K_z, and uniform bounds on K_z, follow from bounds

$$\begin{aligned}\|e^{-zH}\|_{1\to\infty} &\leqslant \left\|e^{-(t/2)H}\right\|_{2\to\infty}\|e^{-isH}\|_{2\to2}\left\|e^{-(t/2)H}\right\|_{1\to2}\\ &\leqslant \left(\left\|e^{-(t/2)H}\right\|_{2\to\infty}\right)^2 \leqslant c\,t^{-D/2} = c\,(\operatorname{Re} z)^{-D/2}\end{aligned}$$

where $z = t + is$ with $t > 0$, $s \in \mathbf{R}$. Then the lemma is obtained by a complex-analytic argument as in [**3**, Theorem 3.4.8]. □

For $\lambda \in \mathbf{C} - (-\infty, 0]$ we let $R_\lambda(\cdot\,;\cdot)$ denote the integral kernel of $(\lambda I + H)^{-1}$.

Lemma 5. *For any $\rho \in [0, \pi)$, and any $q > 1$, there is a $c = c(\rho, q) > 0$ such that*

$$\left|R_\lambda(x\,;y)\right| \leqslant c\,d^{-D+2}e^{-|\lambda|^{1/2}q^{-1}\cos(\theta/2)d}$$

for all $\lambda \in \mathbf{C} - \{0\}$ with $\theta = \arg\lambda \in [-\rho, \rho]$ and all $x, y \in X$.

Proof: Write $\lambda = Re^{i\theta}$ where $R > 0$, $\theta \in [0, \rho]$. (Because of the reflection relation $R_{\overline{\lambda}}(x, y) = \overline{R_\lambda(y, x)}$, it is sufficient to prove the lemma for such θ.) Let $\tau \in [0, \pi/2)$ be such that $0 \leqslant \theta - \tau < \pi/2$, and set $\lambda' = Re^{i\tau}$. Then

$$(\lambda I + H)^{-1} = e^{-i(\theta-\tau)}\left(\lambda' I + e^{-i(\theta-\tau)}H\right)^{-1} = e^{-i(\theta-\tau)}\int_0^\infty dt\,e^{-\lambda' t}\,S_{te^{-i(\theta-\tau)}}\quad .$$

Thus applying Lemma 4, and a change of variable $s = d^{-2}t$,

$$\begin{aligned}\left|R_\lambda(x\,;y)\right| &\leqslant \int_0^\infty dt\,|e^{-\lambda' t}|\left|K_{te^{-i(\theta-\tau)}}(x\,;y)\right|\\ &\leqslant \int_0^\infty dt\,e^{-Rt\cos\tau}c_r\left(t\cos(\theta-\tau)\right)^{-D/2}e^{-(4r)^{-1}\cos(\theta-\tau)(d^2/t)}\\ &= c_r\left(\cos(\theta-\tau)\right)^{-D/2}d^{-D+2}\int_0^\infty ds\,s^{-D/2}e^{-Rd^2s\cos\tau-(4r)^{-1}\cos(\theta-\tau)s^{-1}}\\ &= c_r\left(\cos(\theta-\tau)\right)^{-D/2}d^{-D+2}\\ &\quad\cdot\int_0^\infty ds\,s^{-D/2}e^{-Rd^2s\cos\tau-\delta(4r)^{-1}\cos(\theta-\tau)s^{-1}}e^{-(1-\delta)(4r)^{-1}\cos(\theta-\tau)s^{-1}}\end{aligned}$$

for arbitrary $r > 1$ and $\delta \in (0, 1)$. But for every $s > 0$, one has

$$Rd^2s\cos\tau + \delta(4r)^{-1}\cos(\theta-\tau)s^{-1} \geqslant (R\delta/r)^{1/2}\left(\cos\tau\cos(\theta-\tau)\right)^{1/2}d$$

and hence

$$\left|R_\lambda(x\,;y)\right| \leqslant c_\tau \left(\cos(\theta-\tau)\right)^{-D/2} d^{-D+2}\exp\left(-(R\delta/r)^{1/2}\left(\cos\tau\cos(\theta-\tau)\right)^{1/2} d\right) \cdot \int_0^\infty ds\, s^{-D/2} e^{-(1-\delta)(4r)^{-1}\cos(\theta-\tau)s^{-1}} .$$

Now choose $\tau = \theta/2$ to maximise the function $\tau \mapsto \cos\tau\cos(\theta-\tau)$ on $[0,\theta]$. Since r and δ may be chosen arbitrarily close to 1, the lemma follows. $\square$

Henceforth we assume x, y and $t > 0$ are such that $d(x\,;y) \geqslant t^{1/m}$ and prove the bounds of Theorem 1 under this assumption. This will complete the proof of Theorem 1, since the bounds for $d(x\,;y) \leqslant t^{1/m}$ follow from Lemma 2.

Let $\sigma \in (\pi/2, \pi)$ and $R > 0$ and define the contour $\Gamma = \Gamma(R,\sigma)$ in the complex plane by $\Gamma = L_+ \cup A \cup L_-$, where $L_\pm = \left\{\lambda \in \mathbf{C} : \arg\lambda = \pm\sigma, |\lambda| \geqslant R\right\}$ and $A = \left\{\lambda \in \mathbf{C} : |\arg\lambda| \leqslant \sigma, |\lambda| = R\right\}$. Here Γ is oriented to run along L_- towards the origin, then anti-clockwise around A and along L_+ away from the origin. Then one has the Cauchy integral representation

$$S_t^{(m)} = \frac{1}{2\pi i}\int_\Gamma d\lambda\, e^{\lambda t}(\lambda I + H^n)^{-1}$$

where $n = m/2$ (see [**2**, Section 2.5], or [**9**, Chapter IX]). If $\lambda \in \mathbf{C} - \{0\}$ and $\alpha \in (0,1)$ define $\lambda^\alpha = |\lambda|^\alpha e^{i\alpha\arg\lambda}$ and let $-\lambda_1, \dots, -\lambda_n$ be the n-th roots of $-\lambda$. More precisely, let $\lambda_k = -e^{-\pi i/n}\lambda^{1/n}\omega^k$ for $k \in \{1,\dots,n\}$, where $\omega = e^{2\pi i/n}$. Then one has the partial fraction decomposition

$$(\lambda I + H^n)^{-1} = (\lambda_1 I + H)^{-1}\dots(\lambda_n I + H)^{-1} = \sum_{k=1}^n c_k\left(\lambda^{1/n}\right)^{1-n}(\lambda_k I + H)^{-1}$$

where one may calculate $c_k = -e^{-\pi i/n}\prod_{1\leqslant l\leqslant n, l\neq k}\left(\omega^k - \omega^l\right)^{-1}$. Combining this with the Cauchy integral representation yields

$$\left|K_t^{(m)}(x\,;y)\right| \leqslant (2\pi)^{-1}\sum_{k=1}^n |c_k|\int_\Gamma d|\lambda|\,|e^{\lambda t}||\lambda|^{-1+(1/n)}\left|R_{\lambda_k}(x\,;y)\right| . \tag{3}$$

We shall use Lemma 5 to bound the right hand side. First observe that if $\lambda \in \mathbf{C} - \{0\}$ and the λ_k are as above, then $\pi - |\arg\lambda_k| \geqslant \left(\pi - |\theta|\right)/n$, where $\theta = \arg\lambda$. Hence $|\arg\lambda_k|/2 \leqslant (\pi/2) - \left(\pi - |\theta|\right)/m$ and

$$\cos\left((\arg\lambda_k)/2\right) \geqslant \cos\left(\pi/2 - \left(\pi - |\theta|\right)/m\right) = \sin\left(\left(\pi - |\theta|\right)/m\right) . \tag{4}$$

Also, $|\lambda_k| = |\lambda|^{1/n}$. Therefore by Lemma 5, for an arbitrary $q > 1$ there is an $a > 0$, depending on q and σ, such that

$$\int_A d|\lambda|\,|e^{\lambda t}||\lambda|^{-1+(1/n)}\left|R_{\lambda_k}(x\,;y)\right| \leqslant a\int_{-\sigma}^{\sigma} d\theta\, Re^{Rt\cos\theta}R^{-1+(1/n)}d^{-D+2}e^{-q^{-1}R^{1/m}\sin((\pi-|\theta|)/m)d}$$
$$= 2a\,d^{-D+2}R^{1/n}\int_0^\sigma d\theta\, e^{Rt\cos\theta - q^{-1}R^{1/m}\sin((\pi-\theta)/m)d} .$$

Now choose $R = (qm)^{-m/(m-1)}(d/t)^{m/(m-1)}$ and use the assumptions $D \geqslant 4$ and $d \geqslant t^{1/m}$ to obtain

$$(5)\quad \int_A d|\lambda|\, |e^{\lambda t}| |\lambda|^{-1+(1/n)} \left|R_{\lambda_k}(x\,;y)\right| \leqslant a_1\, t^{-D/m} \int_0^\sigma d\theta\, e^{-(qm)^{-m/(m-1)}\, G(\theta)(d^m/t)^{1/(m-1)}},$$

where a_1 depends on q and σ, and $G(\theta) = m \sin\big((\pi - \theta)/m\big) - \cos\theta$ for $0 \leqslant \theta \leqslant \pi$. Let $\delta \in (0,1)$ be arbitrary. To estimate the integral over $L_\pm$ we use Lemma 5, (4) and our choice of R:

$$\begin{aligned}
\int_{L_\pm} d|\lambda|\, |e^{\lambda t}| |\lambda|^{-1+(1/n)} \left|R_{\lambda_k}(x,y)\right| &\leqslant \int_R^\infty d\tau\, e^{\tau t \cos\sigma} \tau^{-1+(1/n)}\, a\, d^{-D+2} e^{-q^{-1}\tau^{1/m} \sin((\pi-\sigma)/m) d} \\
&\leqslant a\, d^{-D+2} \exp\left(\delta \left\{Rt\cos\sigma - q^{-1} R^{1/m} \sin\left(\frac{\pi-\sigma}{m}\right) d\right\}\right) \\
&\qquad \cdot \int_R^\infty d\tau\, e^{(1-\delta)\tau t \cos\sigma} \tau^{-1+(1/n)} \\
&\leqslant a\, d^{-D+2} \exp\left(\delta \left\{Rt\cos\sigma - q^{-1} R^{1/m} \sin\left(\frac{\pi-\sigma}{m}\right) d\right\}\right) \\
&\qquad \cdot t^{-1/n} \int_0^\infty d\nu\, e^{(1-\delta)\nu \cos\sigma} \nu^{-1+(1/n)} \\
(6)\qquad &\leqslant a_2\, t^{-D/m}\, e^{-(qm)^{-m/(m-1)}\, \delta\, G(\sigma)(d^m/t)^{1/(m-1)}}
\end{aligned}$$

where $a_2 = a \int_0^\infty d\nu\, e^{(1-\delta)\nu\cos\sigma} \nu^{-1+(1/n)}$ depends on q, σ and δ. Next we minimise G.

LEMMA 6. *Let* $\theta_0 = (m-2)\pi/(2m-2)$, $\theta_1 = (m+2)\pi/(2m+2)$. *Then* $G(\theta) \geqslant (m-1)\sin\big(\pi/(2m-2)\big)$ *for all* $\theta \in [0, \theta_1]$, *with equality if and only if* $\theta = \theta_0$.

PROOF: Elementary calculations show that, for $0 \leqslant \theta \leqslant \pi$, $G'(\theta) = 0$ precisely if $\theta = \theta_0$ or $\theta = \theta_1$, and that $G'(\theta) < 0$ for $0 \leqslant \theta < \theta_0$ while $G'(\theta) > 0$ for $\theta_0 < \theta < \theta_1$. Since $G(\theta_0) = (m-1)\sin\big(\pi/(2m-2)\big)$, the proof is complete. ∎

Now in the path of integration $\Gamma = \Gamma(R,\sigma) = \Gamma\big((qm)^{-m/(m-1)}(d/t)^{m/(m-1)}, \sigma\big)$ we fix a choice $\sigma \in (\pi/2, \theta_1]$. By combining (3), (5) and (6), and applying Lemma 6, we obtain

$$\begin{aligned}
\left|K_t^{(m)}(x\,;y)\right| &\leqslant (2\pi)^{-1} \sum_{k=1}^n |c_k| \Big(a_1 \sigma\, t^{-D/m}\, e^{-q^{-m/(m-1)}\, b_m (d^m/t)^{1/(m-1)}} \\
&\qquad\qquad + 2a_2\, t^{-D/m}\, e^{-q^{-m/(m-1)}\, \delta\, b_m (d^m/t)^{1/(m-1)}}\Big) \\
&\leqslant a_3\, t^{-D/m}\, e^{-q^{-m/(m-1)}\, \delta\, b_m (d^m/t)^{1/(m-1)}}
\end{aligned}$$

where $a_3 = (2\pi)^{-1}(a_1\sigma + 2a_2) \sum_{k=1}^n |c_k|$ depends on q, σ and δ. Since $q > 1$ and $\delta \in (0,1)$ may be chosen arbitrarily close to 1, the proof of Theorem 1 is complete.

3. POWERS OF THE LAPLACIAN ON $\mathbf{R}^N$

If α is a multi-index, and ζ a vector in $\mathbf{R}^N$ or $\mathbf{C}^N$, we use the standard notations ∂^α for $\partial_1^{\alpha_1} \ldots \partial_N^{\alpha_N}$, $|\alpha|$ for $\alpha_1 + \cdots + \alpha_N$ and ζ^α for $\zeta_1^{\alpha_1} \ldots \zeta_N^{\alpha_N}$. Moreover $|x|$ denotes the

Euclidean norm of $x \in \mathbf{R}^N$. We consider the operator $H = \Delta^{m/2}$ acting on $L^2(\mathbf{R}^N)$, where m is a fixed positive even integer with $m \geqslant 4$. The symbol of H is the polynomial $P(\zeta) = \left(\sum_{j=1}^{N} \zeta_j^2\right)^{m/2}$ defined for $\zeta \in \mathbf{C}^N$. Then H corresponds in Fourier space to multiplication by $\xi \in \mathbf{R}^N \mapsto P(\xi) = |\xi|^m$. The kernel $K^{(m)}$ of the corresponding semigroup $S_t = e^{-tH}$ is given by $K_t^{(m)}(x\,;y) = L_t(x-y)$, where

$$L_t(x) = (2\pi)^{-N} \int_{\mathbf{R}^N} d\xi\, e^{-tP(\xi)} e^{ix\cdot\xi} \quad , \quad x \in \mathbf{R}^N. \tag{7}$$

Our aim in this section is to prove

THEOREM 7. (I) *The kernel satisfies bounds*

$$\left|L_t(x)\right| \leqslant c\, t^{-N/m} e^{-b_m(|x|^m/t)^{1/(m-1)}}$$

for all $x \in \mathbf{R}^N$ and $t > 0$, where b_m is given by (2) and $c > 0$ is a constant depending only on m and N.
(II) *The coefficient b_m in these bounds is optimal, that is, the bounds are not valid if b_m is replaced by any b with $b > b_m$.*

We shall prove part (I) first. It is convenient to introduce the function $\sigma : (0,\infty) \to (0,\infty)$ defined by $\sigma(k) = m^{-1}(m-1)(km)^{-1/(m-1)}$. Then note that $\inf\{\, k\lambda^m t - \lambda\rho : \lambda > 0\} = -\sigma(k)\,(\rho^m/t)^{1/(m-1)}$ for each $t > 0$, $\rho \geqslant 0$ and $k > 0$. Also observe that if we define

$$k_m = \left(\sin\left(\pi/(2m-2)\right)\right)^{-m+1}$$

then $\sigma(k_m) = b_m$.

In the following preliminary lemma we write $\left\|(s,t)\right\|$ for $(s^2+t^2)^{1/2}$.

LEMMA 8. *The polynomial $Q(s,t) = \mathrm{Re}\left((s+i)^2 + t^2\right)^{m/2}$, $s,t \in \mathbf{R}$, has absolute minimum $-k_m$ achieved at precisely two points $(s,t) = (\pm s_m, 0)$, where $s_m > 0$ depends only on m. There exist $c_1, c_2 > 0$ such that*

$$Q(s,t) = -k_m + c_1(s-s_m)^2 + c_2 t^2 + O\left(\left\|(s-s_m,t)\right\|^3\right) \quad \text{as } (s,t) \to (s_m,0)\,,$$
$$Q(s,t) = -k_m + c_1(s+s_m)^2 + c_2 t^2 + O\left(\left\|(s+s_m,t)\right\|^3\right) \quad \text{as } (s,t) \to (-s_m,0)\,.$$

Moreover, for any $\delta > 0$ there exists a $K_\delta > 0$ such that

$$Q(s,t) \geqslant -k_m + K_\delta\,\left(s^2+t^2\right)^{m/2}$$

for all (s,t) such that $\left\|(s-s_m,t)\right\| \geqslant \delta$ and $\left\|(s+s_m,t)\right\| \geqslant \delta$.

PROOF: To minimise $s \mapsto Q(s,0) = \mathrm{Re}\,(s+i)^m$ one sets $s + i = \mu e^{i\theta}$, $\mu > 0$, $0 < \theta < \pi$, as in [1]. Then $\mu^2 = \sin^{-2}\theta$ and $Q(s,0) = S(\theta) := \sin^{-m}\theta\,\cos(m\theta)$.

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By elementary calculus one finds that S achieves an absolute minimum $-k_m$, precisely at the points $\theta = \theta_m, \theta = \pi - \theta_m$, where $\theta_m = \pi/(2m-2)$. Furthermore, $S''(\theta_m) = S''(\pi - \theta_m) > 0$. Thus $S(\theta) = -k_m + (1/2)S''(\theta_m)(\theta - \theta_m)^2 + O\left((\theta - \theta_m)^3\right)$ as $\theta \to \theta_m$, with a similar expression for θ close to $\pi - \theta_m$. Next consider $\tilde{Q}(\theta, t) := Q(s,t)$: by expanding the brackets in the definition of Q, one finds that $\tilde{Q}$ is the sum of $S(\theta)$ and terms in $t^2, t^4, \ldots, t^m$ whose coefficients depend on θ. In particular, explicit calculation shows that the coefficient of t^2 is positive when evaluated at $\theta = \theta_m$ (or $\theta = \pi - \theta_m$). Upon changing back from θ to s, this leads to the expansions of Q near $(\pm s_m, 0)$, where $s_m + i = \sin^{-1}(\theta_m)e^{i\theta_m}$.

Next, by calculating $\partial Q/\partial s$, $\partial Q/\partial t$ one finds that the only stationary points (s_0, t_0) of Q with $t_0 \neq 0$ are $(s_0, t_0) = (0, \pm 1)$. Since $Q(0, \pm 1) = 0$ and $Q(s,t) \to \infty$ as $\left\|(s,t)\right\| \to \infty$ it follows that $-k_m$ is indeed the absolute minimum of Q.

Since $Q(s,t)$ is the sum of $(s^2+t^2)^{m/2}$ and terms which have lower degree in s and t, the final statement of the lemma certainly holds when $\left\|(s,t)\right\|$ is large enough, say when $\left\|(s,t)\right\| \geqslant R$. Because $Q(s,t) + k_m > 0$ when $(s,t) \neq (\pm s_m, 0)$, a simple compactness argument yields the statement for $\left\|(s,t)\right\| \leqslant R$ satisfying $\left\|(s \pm s_m, t)\right\| \geqslant \delta$. □

For any $a \in S^{N-1} = \left\{x \in \mathbf{R}^N : |x| = 1\right\}$ define the polynomial P_a by $P_a(\xi) = \operatorname{Re} P(\xi + ia)$ for $\xi \in \mathbf{R}^N$. In [**1**, Lemma 7], Barbatis and Davies identified $-k_m$ as the minimum value of P_a. We also require lower bounds on P_a near the points where the minimum is achieved.

LEMMA 9. *The function $\xi \in \mathbf{R}^N \mapsto P_a(\xi)$ has absolute minimum $-k_m$, attained only at the points $\pm s_m a$ for s_m as in Lemma 8. Moreover there exist $\delta > 0$ and $K > 0$, depending only on m and N, such that*

$$\left.\begin{aligned} P_a(\xi) &\geqslant -k_m + K|\xi - s_m a|^2\,, \quad |\xi - s_m a| \leqslant \delta\,, \\ P_a(\xi) &\geqslant -k_m + K|\xi + s_m a|^2\,, \quad |\xi + s_m a| \leqslant \delta\,. \end{aligned}\right\} \tag{8}$$

Let $F_a = \left\{\xi \in \mathbf{R}^N : |\xi - s_m a| \geqslant \delta, |\xi + s_m a| \geqslant \delta\right\}$. Then there is $K' > 0$ depending only on m, N and δ such that

$$P_a(\xi) \geqslant -k_m + K'|\xi|^m \tag{9}$$

for all $a \in S^{N-1}$ and $\xi \in F_a$.

PROOF: In the case $N = 1$, one has $a = \pm 1$ and $P_{\pm 1}(\xi) = \operatorname{Re}(\xi \pm i)^m$, so the lemma follows by applying Lemma 8 with $s = \pm \xi$ and $t = 0$.

If $N \geqslant 2$, given $a \in S^{N-1}$ one can uniquely decompose any $\xi \in \mathbf{R}^N$ as $\xi = sa + \xi'$, where s is real and ξ' is a vector orthogonal to a. Setting $t = |\xi'|$, simple calculations show that $P_a(\xi) = Q(s,t)$, $|\xi - s_m a|^2 = (s - s_m)^2 + t^2$, $|\xi|^2 = s^2 + t^2$, et cetera, and again the required results follow from Lemma 8. □

The key to obtaining Gaussian bounds on L_t is to shift the contour of integration in (7) (this technique was previously used in [**6**, Proposition I.5.3]. By Cauchy's theorem one may replace ξ by $\xi + i\lambda a$ in (7), for arbitrary $\lambda > 0$ and $a \in S^{N-1}$, yielding

$$L_t(x) = c \int_{\mathbf{R}^N} d\xi \, e^{-tP(\xi+i\lambda a)} e^{ix\cdot\xi} e^{-\lambda a\cdot x} = c \int_{\mathbf{R}^N} d\xi \, e^{-t\lambda^m P((\xi/\lambda)+ia)} e^{ix\cdot\xi} e^{-\lambda a\cdot x}$$

where $c = (2\pi)^{-N}$. Now we apply (9) and the following consequence of (8): there is $K'' > 0$ such that

$$P_a(\xi) \geqslant -k_m + K''|\xi \pm s_m a|^m$$

whenever $|\xi \pm s_m a| \leqslant \delta$. Thus

$$\begin{aligned} \left|L_t(x)\right| &\leqslant c \int d\xi \, e^{-t\lambda^m P_a(\xi/\lambda)} e^{-\lambda a\cdot x} \\ &\leqslant c \int_{\{\xi : |(\xi/\lambda) - s_m a| \leqslant \delta\}} d\xi \, e^{-t\lambda^m K''|(\xi/\lambda) - s_m a|^m} e^{k_m \lambda^m t - \lambda a\cdot x} \\ &\qquad + c \int_{\{\xi : |(\xi/\lambda) + s_m a| \leqslant \delta\}} d\xi \, e^{-t\lambda^m K''|(\xi/\lambda) + s_m a|^m} e^{k_m \lambda^m t - \lambda a\cdot x} \\ &\qquad + c \int_{\{\xi : \xi/\lambda \in F_a\}} d\xi \, e^{-t\lambda^m K'|\xi/\lambda|^m} e^{k_m \lambda^m t - \lambda a\cdot x} . \end{aligned}$$

By changes of variable $\eta = \xi - \lambda s_m a$, $\eta = \xi + \lambda s_m a$ in the first two integrals we obtain

$$\left|L_t(x)\right| \leqslant c \, e^{k_m \lambda^m t - \lambda a\cdot x} \left\{ 2 \int_{\mathbf{R}^N} d\eta \, e^{-K'' t|\eta|^m} + \int_{\mathbf{R}^N} d\xi \, e^{-K' t|\xi|^m} \right\} = c' \, t^{-N/m} e^{k_m \lambda^m t - \lambda a\cdot x} .$$

The proof of part (I) is completed by setting $a = x/|x|$ (or letting $a \in S^{N-1}$ be arbitrary if $x = 0$) and minimising over $\lambda > 0$.

We turn to the proof of (II). Following [**1**], let $\mathcal{E}$ be the set of linear functions $\phi : \mathbf{R}^N \to \mathbf{R}$ of the form $\phi(x) = a \cdot x$, where $a \in S^{N-1}$. For $\lambda \in \mathbf{R}$ and $\phi \in \mathcal{E}$, we define perturbed operators and semigroups by $H_{\lambda\phi} = e^{-\lambda\phi} H e^{\lambda\phi}$ and $S_t^{\lambda\phi} = e^{-\lambda\phi} S_t e^{\lambda\phi}$. The crucial observation of [**1**] is that the operators $H_{\lambda\phi}$ are constant-coefficient differential operators and so can be analyzed using the Fourier transform.

Lemma 10. *For $\phi \in \mathcal{E}$ with $\phi(x) = a \cdot x$, and all $\lambda \in \mathbf{R}$ and $t > 0$,*

$$\|S_t^{\lambda\phi}\|_{2\to 2} = e^{k_m \lambda^m t} .$$

Proof: In this proof we write $P(\zeta) = \sum_{|\alpha|=m} c_\alpha (i\zeta)^\alpha$ and $H = \sum_{|\alpha|=m} c_\alpha \partial^\alpha$ for certain real constants c_α. For a multi-index α, and f in Schwartz space, a straightforward calculation shows that

$$e^{-\lambda\phi} \partial^\alpha e^{\lambda\phi} f = \sum_{\beta+\gamma=\alpha} c_{\beta\gamma} (\lambda a)^\gamma \left(\partial^\beta f\right) , \quad c_{\beta\gamma} = \frac{(\beta+\gamma)!}{\beta!\gamma!} ,$$

where $\beta! = \beta_1! \dots \beta_N!$. Hence $H_{\lambda\phi} = \sum_{|\alpha|=m} c_\alpha \sum_{\beta+\gamma=\alpha} c_{\beta\gamma}(\lambda a)^\gamma \partial^\beta$ so $H_{\lambda\phi}$ corresponds in Fourier space to multiplication by

$$\sum_{|\alpha|=m} c_\alpha \sum_{\beta+\gamma=\alpha} c_{\beta\gamma}(\lambda a)^\gamma (i\xi)^\beta = \sum_{|\alpha|=m} c_\alpha \Big(i\,(\xi - i\lambda a)\Big)^\alpha = P(\xi - i\lambda a)$$

regarded as a function of $\xi \in \mathbf{R}^N$. Hence $S_t^{\lambda\phi}$ corresponds to multiplication by $\xi \mapsto e^{-tP(\xi - i\lambda a)}$. Thus if $\lambda \neq 0$, Lemma 9 gives

$$\|S_t^{\lambda\phi}\|_{2\to 2} = \sup_{\xi\in\mathbf{R}^N} \left| e^{-t\lambda^m P((\xi/\lambda)-ia)} \right| = e^{k_m \lambda^m t} \quad ,$$

and similarly $\left\|S_t\right\|_{2\to 2} = 1$ if $\lambda = 0$. □

Now suppose that L_t satisfies Gaussian bounds with a factor b, $b > b_m$, replacing b_m in the exponential. Choose b' with $b_m < b' < b$ and set $\varepsilon = b - b'$. Define $k' > 0$ by $\sigma(k') = b'$ where the function σ was introduced previously. Then $-b'\,(\rho^m/t)^{1/(m-1)} \leqslant k'\lambda^m t - |\lambda|\rho$ for all $t > 0$, $\rho \geqslant 0$ and $\lambda \in \mathbf{R}$. Thus

$$\begin{aligned} \left|L_t(x-y)\right| &\leqslant c\,t^{-N/m} e^{-b'(|x-y|^m/t)^{1/(m-1)}} e^{-\varepsilon(|x-y|^m/t)^{1/(m-1)}} \\ &\leqslant c\,t^{-N/m} e^{k'\lambda^m t - |\lambda||x-y|} e^{-\varepsilon(|x-y|^m/t)^{1/(m-1)}} \end{aligned}$$

for all $\lambda \in \mathbf{R}$ and $x, y \in \mathbf{R}^N$. Since $S_t^{\lambda\phi}$ has the kernel $K_t^{\lambda\phi}(x\,;y) = e^{-\lambda\phi(x)} L_t(x-y) e^{\lambda\phi(y)}$ and $\left|\phi(x) - \phi(y)\right| \leqslant |x - y|$ we obtain

$$\left|K_t^{\lambda\phi}(x\,;y)\right| \leqslant c\,t^{-N/m} e^{k'\lambda^m t} e^{-\varepsilon(|x-y|^m/t)^{1/(m-1)}} \quad ,$$

and it follows that

$$\left\|S_t^{\lambda\phi}\right\|_{\infty\to\infty} = \sup_{x\in\mathbf{R}^N} \int dy \left|K_t^{\lambda\phi}(x\,;y)\right| \leqslant c'\, e^{k'\lambda^m t} \quad .$$

Here c' is a constant which does not depend on t, λ or ϕ. By duality, $\|S_t^{\lambda\phi}\|_{1\to 1} \leqslant c'\,e^{k'\lambda^m t}$ and by interpolation one finds $\left\|S_t^{\lambda\phi}\right\|_{2\to 2} \leqslant c'\,e^{k'\lambda^m t}$. But $\sigma(k') = b' > b_m = \sigma(k_m)$ implies that $k' < k_m$, so this contradicts Lemma 10 when $\lambda^m t$ is sufficiently large. Thus the Gaussian bounds with $b > b_m$ are impossible.

REMARK. Theorem 7 may be extended to a larger class of operators on $\mathbf{R}^N$. Indeed, consider a homogeneous m-th order operator $H = \sum_{|\alpha|=m} c_\alpha \partial^\alpha$ with constant complex coefficients c_α, where $m \geqslant 4$ is even. Assume that H is strongly elliptic in the sense that $\operatorname{Re} P(\xi) \geqslant \mu|\xi|^m$, $\xi \in \mathbf{R}^N$, for some $\mu > 0$, where $P(\zeta) = \sum_{|\alpha|=m} c_\alpha (i\zeta)^\alpha$, $\zeta \in \mathbf{C}^N$, is the symbol of H. We define $k_{H,a} = -\min_{\xi\in\mathbf{R}^N} \operatorname{Re} P(\xi + ia)$ for each $a \in S^{N-1}$, and set $k_H = \max_{a\in S^{N-1}} k_{H,a}$. Then for each $\varepsilon > 0$ there exists $\mu_\varepsilon > 0$ such that

$$\operatorname{Re} P(\xi + ia) \geqslant \mu_\varepsilon |\xi|^m - k_H - \varepsilon \tag{10}$$

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for all $\xi \in \mathbf{R}^N$ and $a \in S^{N-1}$. (For large $|\xi|$ this follows by using the strong ellipticity condition, while for small $|\xi|$ one uses the definition of k_H.) The kernel $L_t^{(H)}$ of e^{-tH} has a Fourier representation analogous to (7) and by shifting the contour of integration as in the proof of Theorem 7 and applying (10), one obtains bounds

$$\left|L_t^{(H)}(x)\right| \leqslant c_r\, t^{-N/m} e^{-(b_H/r)(|x|^m/t)^{1/(m-1)}} \tag{11}$$

for each $r > 1$, where $b_H = \sigma(k_H)$. It is unclear whether one can choose $r = 1$ in general: this would require a more careful analysis of the polynomials $\operatorname{Re} P(\xi + ia)$ near their minima.

The constant b_H is optimal in the sense that the bounds (11) cannot hold if $0 < r < 1$. The proof of this is similar to the proof of Theorem 7(II), but in place of Lemma 10 one finds that $\|S_t^{\lambda\phi}\|_{2\to2} = e^{k_{H,a}\lambda^m t}$ for $\phi \in \mathcal{E}$ with $\phi(x) = a \cdot x$.

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