

POINTWISE BOUNDS ON THE SPACE AND TIME DERIVATIVES OF HEAT KERNELS

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1. INTRODUCTION

Let $K(t, x, y)$ be the heat kernel of the Laplace-Beltrami operator on a complete Riemannian manifold Ω , and put $H = -\Delta$. Then K is a positive C^∞ function on $(0, \infty) \times \Omega \times \Omega$ and there are a number of very sharp pointwise bounds on K , both upper and lower, now available [6, 7, 12].

The present paper shows how to combine these pointwise bounds with a parabolic Harnack inequality of Li and Yau [12] in order to get pointwise bounds on the first order space derivatives of the heat kernel. Our bounds are close to sharp in many cases, and yield similar bounds on the Green function by a standard integration procedure. Although the techniques involved in their proof are not particularly novel, we present them because such bounds are of importance in a variety of contexts, for example [2], which motivated our present study.

We start by assuming that the heat kernel satisfies bounds of a type which are by now becoming standard. We deal with three cases in turn, the first and simplest in the most detail.

Case 1. We assume that

$$(1.1) \quad 0 \leq K(t, x, x) \leq c_1 t^{-N/2}$$

for all $0 < t < \infty$ and $x \in \Omega$. It is known [6] that this implies

$$(1.2) \quad 0 \leq K(t, x, y) \leq c_\delta t^{-N/2} e^{-d^2/(4+\delta)t}$$

for all $0 < \delta < 1$ and $t > 0$, where d is the Riemannian distance between x and y . Indeed it turns out that $c_\delta = c_0 \delta^{-N/2}$ and this leads to the sharper bound

$$0 \leq K(t, x, y) \leq c t^{-N/2} \left[1 + \frac{d^2}{t} \right]^{N/2} e^{-d^2/4t}.$$

See [10] for details.

Case 2. We assume that

$$(1.3) \quad 0 \leq K(t, x, y) \leq \begin{cases} c_\delta t^{-N/2} e^{-d^2/(4+\delta)t} & \text{if } 0 < t \leq 1 \\ c_\delta t^{-M/2} e^{-d^2/(4+\delta)t} & \text{if } 1 \leq t < \infty \end{cases}$$

for all $0 < \delta < 1$, and some $0 \leq M \leq N$. Such bounds hold with $M = 0$ for compact manifolds, and are also relevant to many complete manifolds with bounded geometry and non-negative Ricci curvature [6, 12]. See also [10] for the sharper bounds possible if one optimises with respect to δ .

Case 3. We assume that

$$0 \leq K(t, x, y) \leq \begin{cases} c_\delta t^{-N/2} e^{-d^2/(4+\delta)t} & \text{if } 0 < t \leq 1 \\ c_\delta e^{(\delta-E)t-d^2/(4+\delta)t} & \text{if } 1 \leq t < \infty \end{cases}$$

for all $0 < \delta < 1$, where $E > 0$ is the bottom of the spectrum of H . Such bounds apply to complete manifolds with bounded geometry and negative Ricci curvature [8]. Indeed for hyperbolic space one may put $\delta = 0$, and get sharp upper and lower bounds in terms of elementary functions [9].

In Section 2 we obtain bounds on $\frac{\partial K}{\partial t}$ in each of the three above cases.

In Section 3 we combine these with the parabolic Harnack inequality of Li and Yau [12] to obtain bounds on the space derivatives. Some consequences of the bounds are also dealt with in Section 3, and in particular a Sobolev imbedding theorem is proved.

2. THE TIME DERIVATIVE

The crucial estimate is an improvement of bounds in [5, 6].

PROPOSITION 1. *Let $f(z)$ be an analytic function defined for $\text{Re } z > 0$, and satisfying*

$$(2.1) \quad \begin{aligned} |f(z)| &\leq a(\text{Re } z)^{-N/2} \quad \text{all } \text{Re } z > 0 \\ |f(r)| &\leq ar^{-N/2} e^{-b/r} \quad \text{all } r > 0 \end{aligned}$$

for some $a > 0$ and $b > 0$. Then

$$|f(re^{i\theta})| \leq aer^{-N/2} \left[2 \sec \theta + \frac{2b}{r} \right]^{2N|\theta|/\pi} \exp(-b \cos \theta/r)$$

for all $r > 0$ and $|\theta| < \pi/2$. Also

$$(2.2) \quad |f'(r)| \leq a c_N r^{-1-N/2} \left[1 + \frac{b}{r} \right] e^{-b/r}$$

for all $r > 0$.

Proof. We suppose that $0 < \gamma < \pi/2$ and that $z = re^{i\theta}$ where $0 \leq \theta \leq \gamma$. If we put

$$g(z) = z^{-N/2} f(z^{-1}) \exp\{be^{i(\pi/2-\gamma)} z/\sin \gamma\}$$

then

$$|g(r)| \leq a, \quad |g(re^{i\gamma})| \leq a(\sec \gamma)^{N/2}.$$

Moreover

$$|g(z)| \leq a(\sec \gamma)^{N/2} \exp \left\{ \frac{br}{\sin \gamma} \right\}$$

throughout the sector. The Phragmén-Lindelöf theorem now implies that

$$|g(z)| \leq a(\sec \gamma)^{N\theta/2\gamma}$$

for all $0 \leq \theta \leq \gamma$. Combining this with a similar bound for $-\gamma \leq \theta \leq 0$ we deduce that

$$|f(z)| \leq ar^{-N/2} (\sec \gamma)^{N\theta/2\gamma} \exp \left\{ \frac{b \sin(\gamma - |\theta|)}{r \sin \gamma} \right\}$$

for all $|\theta| \leq \gamma$. If we now put

$$\gamma = (1 - \varepsilon)\pi/2 + \varepsilon|\theta|$$

where $0 < \varepsilon \leq 1/2$ then $|\theta| < \gamma$ and $\pi/4 \leq \gamma < \pi/2$. Hence

$$\cos \gamma = \sin \left\{ \varepsilon \left(\frac{\pi}{2} - |\theta| \right) \right\} \geq \varepsilon \sin \left(\frac{\pi}{2} - |\theta| \right) = \varepsilon \cos \theta,$$

$$\sin(\gamma - |\theta|) = \sin \left\{ (1 - \varepsilon) \left(\frac{\pi}{2} - |\theta| \right) \right\} \geq$$

$$\geq (1 - \varepsilon) \sin \left(\frac{\pi}{2} - |\theta| \right) = (1 - \varepsilon) \cos \theta,$$

and

$$N|\theta|/2\gamma \leq 2N|\theta|/\pi.$$

These yield

$$|f(z)| \leq ar^{-N/2}(e^{-1}\sec\theta)^{N\theta/\pi}\exp(-b(1-\varepsilon)\cos\theta/r).$$

We now substitute

$$\varepsilon = \frac{1}{2} \left[1 + \frac{b \cos \theta}{r} \right]^{-1}$$

into the above formula to obtain the first statement of the theorem.

Next put

$$h(z) = e^{b/z}f(z)$$

so that

$$|h(z)| \leq aer^{-N/2} \left(2\sec\theta + \frac{2b}{r} \right)^{2N\theta/\pi}$$

for all $|\theta| < \pi$, and let γ be the circle with centre $s \in (0, \infty)$ and radius λs where $0 < \lambda < 1$. Then $re^{i\theta} \in \gamma$ implies

$$(1 - \lambda)s \leq r \leq (1 + \lambda)s; \quad |\theta| \leq \sin^{-1}\lambda.$$

Therefore $z \in \gamma$ implies

$$|h(z)| \leq ae(1 - \lambda)^{-N/2}s^{-N/2} \left[2(1 - \lambda^2)^{1/2} + \frac{2b}{(1 - \lambda)s} \right]^{2N\pi^{-1}\sin^{-1}\lambda} = c \text{ (say).}$$

Cauchy's integral formula yields

$$|h'(s)| \leq \frac{c}{\lambda s}$$

so

$$\left| \frac{b}{s^2} e^{b/s}f(s) + e^{b/s}f'(s) \right| \leq \frac{c}{\lambda s}$$

and

$$|f'(s)| \leq \frac{b}{s^2} |f(s)| + \frac{c}{\lambda s} e^{-b/s}.$$

Finally we put

$$\lambda = \sin\left(\frac{\pi}{3N}\right)$$

so $0 < \lambda \leq 1/2$ for $N \geq 2$ and $N\sin^{-1}\lambda/\pi = 1/3$. This yields

$$|f'(s)| \leq as^{-1-N/2} \frac{b}{s} e^{-b/s} + ak_N s^{-1-N/2} \left(1 + \frac{b}{s}\right)^{2/3} e^{-b/s}$$

which implies the second statement of the theorem.

NOTE. By examining the particular case

$$f(z) = az^{-N/2} e^{-b/z}$$

we see that the second bound is essentially optimal.

We apply the above theorem to obtain bounds on the time derivative of the heat kernel in each of the three cases below. Our results are by no means novel, but our bounds have sharper constants than those in [11, 16]. In particular our polynomial correction terms in Theorem 2 and Case 1 of Theorem 6 may be compared with those in [10, 16]; we mention that there are some computational errors in [15] which are not altogether easy to put right by the methods of that paper; see [10] and [16, p. 368].

THEOREM 2. *In Case 1 the heat kernel satisfies*

$$\left| \frac{\partial K}{\partial t} \right| \leq c_N t^{-1-N/2} \left(1 + \frac{d^2}{t}\right)^{1+N/3} e^{-d^2/4t}$$

for all $t > 0$.

Proof. If $\|A\|_{q,p}$ denotes the norm of an operator from L^p to L^q then (1.1) states that

$$\|e^{-Ht}\|_{\infty,1} \leq ct^{-N/2}$$

and implies by interpolation that

$$\|e^{-Ht}\|_{\infty,2} = \|e^{-Ht}\|_{2,1} \leq c^{1/2} t^{-N/4}.$$

Therefore

$$\|e^{-H(t+is)}\|_{\infty,1} \leq \|e^{-Ht/2}\|_{\infty,2} \|e^{-His}\|_{2,2} \|e^{-Ht/2}\|_{2,1} \leq c(t/2)^{-N/2}$$

or

$$(2.3) \quad |K(z, x, y)| \leq c2^{N/2}(\operatorname{Re} z)^{-N/2}$$

for all $\operatorname{Re} z > 0$ and $x, y \in \Omega$. Using (1.2) and (2.3), we may now apply Proposition 1 with $a = c2^{N/2}\delta^{-N/2}$ and $b = d^2/(4 + \delta)$ and $f(z) = K(z, x, y)$. We obtain

$$\left| \frac{\partial K}{\partial t} \right| \leq c2^{N/2}\delta^{-N/2}k_N t^{-1-N/2} \left(1 + \frac{d^2}{t} \right) e^{-d^2/(4+\delta)t}.$$

Putting $\delta = (1 + d^2/t)^{-1}$ we finally obtain the statement of the theorem.

THEOREM 3. *In Case 2 the heat kernel satisfies*

$$\left| \frac{\partial K}{\partial t} \right| \leq \begin{cases} a_{\delta, M, N} t^{-1-N/2} e^{-d^2/(4+\delta)t} & \text{if } 0 < t \leq 1 \\ a_{\delta, M, N} t^{-1-M/2} e^{-d^2/(4+\delta)t} & \text{if } 1 \leq t < \infty. \end{cases}$$

Proof. If $\lambda > 0$ then starting from (1.3), separate calculations for $0 < t \leq 1$ and $1 \leq t < \infty$ yield

$$0 \leq e^{-\lambda t} K(t, x, y) \leq \Gamma \left(\frac{N-M}{2} + 1 \right) c_{\delta} (1 + \lambda^{-1})^{(N-M)/2} t^{-N/2} e^{-d^2/(4+\delta)t}.$$

This implies as before that

$$|e^{-\lambda z} K(z, x, y)| \leq \Gamma \left(\frac{N-M}{2} + 1 \right) c_{\delta} (1 + \lambda^{-1})^{(N-M)/2} 2^{N/2} (\operatorname{Re} z)^{-N/2}$$

so we can proceed as in Theorem 2 but with

$$a = c_{\delta, M, N} (1 + \lambda^{-1})^{(M-N)/2},$$

$$b = d^2/(4 + \delta),$$

$$f(z) = e^{-\lambda z} K(z, x, y).$$

We then obtain

$$\begin{aligned} \left| e^{-\lambda t} \frac{\partial K}{\partial t} - \lambda e^{-\lambda t} K \right| &\leq \\ &\leq c_{\delta, M, N} k_N (1 + \lambda^{-1})^{(N-M)/2} t^{-1-N/2} \left[1 + \frac{d^2}{4t} \right]^{1+N/2} e^{-d^2/(4+\delta)t}. \end{aligned}$$

Putting $\lambda = t^{-1}$ we finally get

$$\left| \frac{\partial K}{\partial t} \right| \leq t^{-1}K + ec_{\delta, M, N}k_N(1+t)^{(N-M)/2}t^{-1-N/2} \left[1 + \frac{d^2}{4t} \right]^{1+N/2} e^{-d^2/(4+\delta)t}.$$

The term $\left[1 + \frac{d^2}{4t} \right]^{1+N/2}$ can be absorbed into $e^{-d^2/(4+\delta)t}$ by increasing the value of δ slightly, and the theorem then follows.

THEOREM 4. *In Case 3 the heat kernel satisfies*

$$\left| \frac{\partial K}{\partial t} \right| \leq \begin{cases} a_{\delta, N, E}t^{-1-N/2}e^{-d^2/(4+\delta)t} & \text{if } 0 < t \leq 1 \\ a_{\delta, N, E}e^{(\delta-E)t-d^2/(4+\delta)t} & \text{if } 1 \leq t < \infty. \end{cases}$$

Proof. We now study

$$e^{(E-\delta-\lambda)t}K(t, x, y).$$

If $\lambda > 0$ and $t > 0$ then

$$0 \leq e^{(E-\delta-\lambda)t}K(t, x, y) \leq c_{\delta} \Gamma\left(\frac{N}{2} + 1\right) (1 + \lambda^{-1})^{N/2} t^{-N/2} e^{-d^2/(4+\delta)t}.$$

If $\lambda > 0$ and $0 < \operatorname{Re} z \leq 1$ then

$$|e^{(E-\delta-\lambda)z}K(z, x, y)| \leq c_{\delta} 2^{N/2} (\operatorname{Re} z)^{-N/2} e^{(E-\lambda)\operatorname{Re} z}.$$

Finally, if $\lambda > 0$ and $\operatorname{Re} z \geq 1$ then

$$\|e^{-Hz}\|_{\infty, 1} \leq \|e^{-H/2}\|_{\infty, 2} \|e^{-H(z-1)}\|_{2, 2} \|e^{-H/2}\|_{2, 1} \leq ae^{-E(\operatorname{Re} z - 1)}.$$

Thus

$$\begin{aligned} |e^{(E-\delta-\lambda)z}K(z, x, y)| &\leq ae^{E-\lambda\operatorname{Re} z} \leq \\ &\leq a\Gamma\left(\frac{N}{2} + 1\right) \lambda^{-N/2} (\operatorname{Re} z)^{-N/2}. \end{aligned}$$

Therefore

$$|e^{(E-\delta-\lambda)z}K(z, x, y)| \leq a_{\delta, N, E} (1 + \lambda^{-1})^{N/2} (\operatorname{Re} z)^{-N/2}$$

for all $\lambda > 0$ and $\operatorname{Re} z > 0$.

The remainder of the proof is as before.

3. THE SPACE DERIVATIVE

The crucial result to derive the space derivative is a parabolic Harnack inequality of Li and Yau [12]. We state this in a slightly numerically improved form, taken from [6].

PROPOSITION 5. *Suppose u is a positive solution of*

$$\frac{\partial u}{\partial t} = \Delta u$$

on the complete Riemannian manifold Ω , which has Ricci curvature $\text{Ric} \geq -\rho$ for some constant $\rho \geq 0$. Then

$$(3.1) \quad u^{-2} |\nabla u|^2 - \alpha u^{-1} \frac{\partial u}{\partial t} \leq \frac{1}{2} N \alpha^2 \left[t^{-1} + \frac{\rho}{2(\alpha - 1)} \right]$$

for all $x \in \Omega$, $t > 0$, $\alpha > 1$.

THEOREM 6. *In Case 1 we have*

$$|\nabla_x K| \leq c_N t^{-N/2} (t^{-1} + \rho)^{1/2} \left(1 + \frac{d^2}{t} \right)^{(1+N)/2} e^{-d^2/4t}.$$

In Case 2 we have

$$|\nabla_x K| \leq \begin{cases} c_{\delta, M, N} t^{-N/2} (t^{-1} + \rho)^{1/2} e^{-d^2/(4+\delta)t} & \text{if } 0 < t \leq 1 \\ c_{\delta, M, N} t^{-M/2} (t^{-1} + \rho)^{1/2} e^{-d^2/(4+\delta)t} & \text{if } 1 \leq t < \infty. \end{cases}$$

In Case 3 we have

$$|\nabla_x K| \leq \begin{cases} c_{\delta, N, E} t^{-N/2} (t^{-1} + \rho)^{1/2} e^{-d^2/(4+\delta)t} & \text{if } 0 < t \leq 1 \\ c_{\delta, N, E} e^{(\delta-E)t} (t^{-1} + \rho)^{1/2} e^{-d^2/(4+\delta)t} & \text{if } 1 \leq t < \infty. \end{cases}$$

Proof. Putting $\alpha = 3/2$ in (3.1) yields

$$\begin{aligned} |\nabla u|^2 &\leq 2u \frac{\partial u}{\partial t} + 2u^2 N (t^{-1} + \rho) \leq \\ &\leq 2 \left\{ \left(u \frac{\partial u}{\partial t} \right)^{1/2} + u N^{1/2} (t^{-1} + \rho)^{1/2} \right\}^2. \end{aligned}$$

Therefore

$$\begin{aligned}
 |\nabla u| &\leq 2^{1/2} \left\{ \left(u \frac{\partial u}{\partial t} \right)^{1/2} + uN^{1/2}(t^{-1} + \rho)^{1/2} \right\} \leq \\
 &\leq 3 \max \left\{ \left(u \frac{\partial u}{\partial t} \right)^{1/2}, uN^{1/2}(t^{-1} + \rho)^{1/2} \right\}.
 \end{aligned}$$

The three cases are now all treated by putting

$$u(t, x) = K(t, x, y)$$

and applying one of the bounds on $\left| \frac{\partial K}{\partial t} \right|$.

Once one has bounds on the heat kernel it is easy to deduce corresponding bounds on the Green function. We present the following as a sample of what is possible.

THEOREM 7. *Suppose that $N \geq 3$, $\text{Ric} \geq 0$ and*

$$0 \leq K(t, x, y) \leq ct^{-N/2}$$

for all $t > 0$. Then the Green function $G(\lambda, x, y)$ of $(\lambda + H)^{-1}$ satisfies

$$0 \leq G(\lambda, x, y) \leq c_\delta d^{2-N} \exp\{-(1 - \delta)\lambda^{1/2}d\}$$

and

$$|\nabla_x G(\lambda, x, y)| \leq c_\delta d^{1-N} \exp\{-(1 - \delta)\lambda^{1/2}d\}$$

for all $\lambda \geq 0$, $x, y \in \Omega$ and $0 < \delta < 1$.

The proof follows [5, Lemma 3].

We finally turn to the L^p behavior of the heat kernel. For the remainder of the section we assume that M is a complete Riemannian manifold with bounded geometry, [6]. Then there exists a constant $\rho \geq 0$ such that $\text{Ric} \geq -\rho$ and there exists a constant $c > 0$ such that

$$0 \leq K(t, x, y) \leq \begin{cases} ct^{-N/2} & \text{if } 0 < t \leq 1 \\ c & \text{if } 1 \leq t < \infty \end{cases}$$

where N is the dimension of M ; see [6] for details. Thus the most general case which can occur for a manifold with bounded geometry is Case 2 with $M = 0$.

THEOREM 8. If Ω is a complete Riemannian manifold with bounded geometry, one has

$$(3.2) \quad \|e^{-Ht}\|_{p,p} \leq 1 \quad \text{if } 0 < t < \infty,$$

$$(3.3) \quad \|He^{-Ht}\|_{p,p} \leq \begin{cases} ct^{-1} & \text{if } 0 < t \leq 1 \\ c & \text{if } t \geq 1, \end{cases}$$

$$(3.4) \quad \|\nabla_x e^{-Ht}\|_{p,p} \leq \begin{cases} ct^{-1/3} & \text{if } 0 < t \leq 1 \\ c & \text{if } t \geq 1 \end{cases}$$

or all $1 \leq p \leq \infty$.

Proof. The statement (3.2) is simply recording the fact that e^{-Ht} is a symmetric Markov semigroup. By duality and interpolation it is sufficient to prove the second and third for $p = 1$, and for this purpose we recall that

$$\|A\|_{1,1} = \text{ess sup}_y \int |A(x, y)| dx$$

for any integral operator A . We finally use a result of Gromov [3] to the effect that the area of the sphere $S(x, r)$ with centre x and radius r is bounded by

$$|S(x, r)| \leq cr^{N-1}e^{Rr}$$

where R depends upon N and ρ , and equals zero if $\rho = 0$. Theorem 3 now yields

$$\|He^{-Ht}\|_{1,1} \leq \int_0^\infty a_\delta t^{-1-N/2} e^{-r^2/(4+\delta)t} r^{N-1} e^{Rr} dr$$

if $0 < t \leq 1$. Putting $\delta = 1$ and $r = t^{1/2}s$ we obtain

$$\|He^{-Ht}\|_{1,1} \leq a_1 t^{-1} \int_0^\infty e^{-s^2/5+Rs} s^{N-1} ds = ct^{-1}.$$

If $t \geq 1$ then

$$\|He^{-Ht}\|_{1,1} \leq \|He^{-H}\|_{1,1} \|e^{-H(t-1)}\|_{1,1} \leq c.$$

The proof of the last part (3.4) of the theorem is similar.

Our next corollary is due to Varopoulos [16] for Lie groups and also manifolds with bounded geometry. Although his equation on p. 353, 1.2 has a misprint (the final t should be replaced by $(1 + \delta)t$) this does not affect his conclusion.

COROLLARY 9. *If Ω is a complete manifold with bounded geometry, then $e^{-(H+\varepsilon)t}$ is a bounded holomorphic semigroup on $L^p(\Omega)$ for all $\varepsilon > 0$ and $1 \leq p \leq \infty$.*

Proof. This follows directly from (3.3) upon applying [4, Theorem 2.39].

COROLLARY 10. *If Ω is a complete manifold with bounded geometry and $1 \leq p \leq \infty$ then*

$$\|\nabla(1 - \Delta)^{-\frac{1}{2}-\varepsilon}\|_{p,p} < \infty$$

for all $\varepsilon > 0$.

Proof. This follows from (3.4) upon using the formula

$$\Gamma(\alpha)(1 + H)^{-\alpha} = \int_0^{\infty} t^{\alpha-1} e^{-t} e^{-Ht} dt.$$

NOTE. If $1 < p < \infty$ then one may set $\varepsilon = 0$ in the above corollary, but we believe that this is not true for $p = 1$. See [1, 13, 14].

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