HEAT KERNEL BOUNDS, CONSERVATION OF PROBABILITY AND THE FELLER PROPERTY

By

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Dedicated to Professor Shmuel Agmon

1. Introduction

If Δ is the Laplace–Beltrami operator of a complete Riemannian manifold, we say that $e^{\Delta t}$ conserves probability if

$$e^{\Delta t}1 = 1 \tag{1.1}$$

for some (equivalently all) $t > 0$. A number of different conditions on the Ricci curvature or volume growth of M which imply this property are known [2, 3, 8, 12–18, 21, 23–27, 29, 30]. We mention particularly that (1.1) holds if

$$\mathrm{vol}[B(p,r)] \le \alpha \ \exp(\beta r^2) \tag{1.2}$$

for some $p \in M, \alpha > 0, \beta > 0$ and all $r > 0$, where $B(p,r)$ is the ball in M with centre p and radius r.

In this paper we rewrite the argument of Gaffney [12] in a more general context, and show that it implies the conservation of probability under the condition (1.2); our calculation is closely related to the approach of [2, 18].

More surprisingly, Gaffney's argument also yields a general L^2 Gaussian upper bound on heat kernels, which has been proved elsewhere by wave equation techniques [5]. By combining this with a local parabolic Harnack inequality, we obtain a pointwise Gaussian upper bound on heat kernels which may be used when the heat semigroup is not ultracontractive in the sense of [9] and one does not have pointwise lower bounds on the Ricci curvature.

We say that $e^{\Delta t}$ has the Feller property if

$$e^{\Delta t}C_0 \subseteq C_0 \tag{1.3}$$

for all $t > 0$, where C_0 is the space of continuous functions on M which vanish at infinity. Conditions for this are given in [3, 8, 18, 24, 25]. We give a new condition

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for the Feller property which does not depend upon lower bounds on the Ricci curvature, but rather upon the behaviour at infinity of a modified injectivity radius.

We develop the theory below for weighted Laplace–Beltrami operators on possibly incomplete Riemannian manifolds. Its application to second order elliptic operators on $\mathcal{R}^N$ is explained in Section 4. We note that our theorems may be extended in a variety of ways, for example to Lipschitz manifolds [28] and to complexes obtained by glueing together pieces of Riemannian manifolds in a locally finite manner. One may also replace $\sigma(x)^2$ in (1.5) and (1.6) below by any other weight provided the quadratic form Q is closable; conditions for this may be found in [1, 6, 11].

We assume that M is a Riemannian manifold which is locally finite in the sense that every ball has finite volume; this property holds if M is complete or is an open set in some larger complete manifold. We define $L^\infty_{\rm loc}$ to be the set of measurable functions on M which are bounded on every ball. We assume that $\sigma > 0$ is a measurable function on M with $\sigma^{\pm 1} \in L^\infty_{\rm loc}$. We write dx for the Riemannian volume element on M and $d(x, y)$ for the Riemannian distance.

We shall be concerned with the operator L on M given formally by

$$Lf = \sigma^{-2}\nabla \cdot (\sigma^2 \nabla f) \tag{1.4}$$

subject to Neumann boundary conditions at every point of the boundary of the completion of M, and Dirichlet boundary conditions at infinity.

There are two ways of dealing with the weight σ when it is not identically one. The first is to consider the unweighted Laplace–Beltrami operator Δ' on $M \times S^2$ with respect to the metric

$$dx^2 + \sigma(x)^2 d\omega^2.$$

Properties of the operator L defined by (1.4) can then be obtained from properties of Δ' by looking at the subspace of rotationally invariant functions. The more direct approach, which we adopt, is to include the weight σ in all the definitions and proofs, and observe that it causes no real problems.

Because of the possible non-differentiability of σ, a direct definition of L using (1.4) is not easy, and we start by considering the quadratic form

$$Q(f) = \int_M |\nabla f|^2 \sigma^2 dx \tag{1.5}$$

and the norm

$$\|f\|^2 = \int_M |f|^2 \sigma^2 dx \tag{1.6}$$

where the initial domain of Q is $W_b^{1,\infty}$; this is defined as the space of continuous functions f of bounded support whose weak first derivatives lie in L^∞.

We define an inner product on the set of boundedly supported vector fields by

$$\langle u, v\rangle = \int_M u(x) \cdot v(x)\sigma(x)^2 dx$$

so that

$$Q(f) = \langle \nabla f, \nabla f\rangle.$$

The form Q is a closable Dirichlet form, and we define L to be the self-adjoint operator associated with its closure $\bar{Q}$. We also define $\bar{\nabla}$ to be the L^2 operator closure of ∇ initially defined on $W_b^{1,\infty}$. It is then known [8, 11] that e^{Lt} is a positivity preserving contraction semi-group on L^p for $1 \leq p \leq \infty$ which is strongly continuous for $1 \leq p < \infty$. Also

$$\mathrm{Dom}((-L)^{1/2}) = \mathrm{Dom}(\bar{Q}) = \mathrm{Dom}(\bar{\nabla}).$$

If $\phi : M \to \mathcal{R}$ is a bounded Lipschitz continuous function it is straightforward to show that $f \in \mathrm{Dom}(\bar{\nabla})$ implies $\phi f \in \mathrm{Dom}(\bar{\nabla})$ and

$$\bar{\nabla}(\phi f) = (\nabla\phi)f + \phi(\bar{\nabla} f).$$

We shall apply this with

$$\phi = e^{\alpha\psi} \tag{1.7}$$

where $\alpha \in \mathcal{R}$ and ψ is a bounded function such that $|\nabla\, \psi| \leq 1$, for example

$$\psi(x) = d(x, A) \wedge n$$

where A is any closed subset of M, and $n > 0$.

We conclude this section by presenting the lemma of Gaffney [12], who only treated the case $\sigma = 1$.

Lemma 1 *If $0 \leq f \in L^2$ and $u_t = e^{Lt}f$ then*

$$\|\phi u_t\|_2 \leq e^{\alpha^2 t}\|\phi f\|_2 \tag{1.8}$$

and

$$I_t \equiv \int_0^t \|\phi\bar{\nabla} u_s\|_2^2 ds \leq 2e^{2\alpha^2 t}\|f\phi\|_2^2$$

for all $t > 0$, and all ϕ of the form (1.7).

Proof We have

$$
\begin{aligned}
\frac{\partial}{\partial t}\|\phi u_t\|_2^2 &= \frac{\partial}{\partial t}\langle \phi u_t, \phi u_t\rangle \\
&= 2\langle \phi L u_t, \phi u_t\rangle \\
&= -2\langle \bar{\nabla} u_t, \bar{\nabla}(\phi^2 u_t)\rangle \\
&= -2\langle \bar{\nabla} u_t, 2\phi u_t \nabla\phi + \phi^2 \bar{\nabla} u_t\rangle \\
&= -2\|\phi \bar{\nabla} u_t\|_2^2 - 4\langle \phi\bar{\nabla} u_t, \alpha\phi u_t \nabla\psi\rangle \\
&\leq -2\|\phi\bar{\nabla} u_t\|_2^2 + 2(\lambda^{-1}\|\phi\bar{\nabla} u_t\|_2^2 + \lambda\alpha^2\|\phi u_t\|_2^2)
\end{aligned}
\tag{1.9}
$$

for all $\lambda > 0$, using $|\nabla\psi| \leq 1$. Putting $\lambda = 1$

$$\frac{\partial}{\partial t}\|\phi u_t\|_2^2 \leq 2\alpha^2\|\phi u_t\|_2^2.$$

This yields (1.8) upon integration.

Putting $\lambda = 2$ in (1.9) yields

$$
\begin{aligned}
\frac{\partial}{\partial t}\|\phi u_t\|_2^2 + \|\phi\bar{\nabla} u_t\|_2^2 &\leq 4\alpha^2\|\phi u_t\|_2^2 \\
&\leq 4\alpha^2 e^{2\alpha^2 t}\|\phi f\|_2^2.
\end{aligned}
$$

Integrating this inequality yields

$$\|\phi u_t\|_2^2 - \|\phi f\|_2^2 + I_t \leq 2(e^{2\alpha^2 t} - 1)\|\phi f\|_2^2$$

and hence

$$\|\phi u_t\|_2^2 + I_t \leq 2e^{2\alpha^2 t}\|\phi f\|_2^2$$

which implies the second statement of the lemma. □

2. Gaussian upper bounds on the heat semigroup

The above lemma already enables us to obtain an L^2 Gaussian upper bound on the heat semigroup. For $\sigma = 1$ such bounds have also been obtained by wave equation techniques [5], [4, p. 199]. We recall that the heat kernel of L is defined by

$$e^{Lt}f(x) = \int_M K(t,x,y)f(y)\sigma(y)^2 dy.$$

We define the σ-dependent volume of a Borel subset E of M by

$$|E| = \int_E \sigma(x)^2 dx = \|\chi_E\|_2^2$$

where χ_E is the characteristic function of E.

Given two disjoint subsets E and F of M and a function ψ on M with $|\nabla\psi| \le 1$ we define

$$\psi(E,F) = \inf\{\psi(x) : x \in F\} - \sup\{\psi(x) : x \in E\}$$

and observe that

$$\sup_{\psi} \psi(E,F) = d(E,F) \equiv \inf\{d(x,y) : x \in E, y \in F\}.$$

Theorem 2 *If E and F are two Borel subsets of M with $|E| < \infty$ and $|F| < \infty$, then*

$$0 \le \langle e^{Lt}\chi_E, \chi_F\rangle \le |E|^{1/2}|F|^{1/2}\exp[-d(E,F)^2/4t]$$

for all $t > 0$.

Proof If we put $\psi(x) = d(x,E)$ and $\phi = e^{\alpha\psi}$ then Lemma 1 yields

$$\begin{aligned} 0 &\le \langle e^{Lt}\chi_E, \chi_F\rangle \\ &= \langle \phi e^{Lt}\chi_E, \phi^{-1}\chi_F\rangle \\ &\le e^{\alpha^2 t}\|\phi\chi_E\|_2\|\phi^{-1}\chi_F\|_2 \\ &\le e^{\alpha^2 t}|E|^{1/2}e^{-\alpha d(E,F)}|F|^{1/2}. \end{aligned}$$

This yields the stated result upon putting

$$\alpha = d(E,F)/2t.$$

□

A standard method of passing from L^2 estimates such as Theorem 2 to pointwise bounds is to rely upon suitable Sobolev embedding theorems [5]. These however are only valid if the manifold and metric are sufficiently smooth, and certainly cannot be applied to Lipschitz manifolds. We instead make assumptions on the local geometry expressed in terms of a Harnack inequality. If $\sigma = 1$ this idea has already been exploited in [4, p. 196] and [5]. The simplest form of this is as follows.

(H1) We assume that one is given constants $c(x,s)$ for $x \in M$ and $s > 0$ such that if u is a positive solution of

$$\frac{\partial u}{\partial t} = \sigma^{-2}\nabla \cdot (\sigma^2\nabla u)$$

on $M \times (0, \infty)$ then

$$0 \leq u(x,t) \leq \frac{c(x,s)}{|B(x,s^{1/2})|} \int_{B(x,s^{1/2})} u(y,t+s)\sigma(y^2)dy$$

for all $t > s > 0$ and all $x \in M$.

Theorem 3 *Under the hypothesis* (H1) *we have the pointwise upper bound*

$$0 \leq K(t,x,y) \leq \frac{c(x,s_1)}{|B(x,s_1^{1/2})|^{1/2}} \frac{c(y,s_2)}{|B(y,s_2^{1/2})|^{1/2}} \exp\left[-\frac{(d(x,y) - s_1^{1/2} - s_2^{1/2})_+^2}{4(t+s_1+s_2)} \right]$$

for all $x, y \in M$ and $t > 0$, provided $0 < s_i \leq t$.

Note The best choice of s_1 and s_2 in this inequality will depend upon the particular forms of $c(x,s)$ and $|B(x,s^{1/2})|$ as functions of x and s.

Proof Since $K(t,x,y)$ is a solution of the heat equation as a function of x and t we have

$$K(t,x,y) \leq \frac{c(x,s_1)}{|B(x,s_1^{1/2})|} \int_{B(x,s_1^{1/2})} K(t+s_1,w,y)\sigma^2(w)dw.$$

Since

$$u(y,t) = \int_{B(x,s_1^{1/2})} K(t+s_1,w,y)\sigma^2(w)dw$$

is also a solution of the heat equation we have

$$u(y,t) \leq \frac{c(y,s_2)}{|B(y,s_2^{1/2})|} \int_{B(y,s_2^{1/2})} u(z,t+s_2)\sigma^2(z)dz.$$

Combining these estimates we obtain

$$K(t,x,y) \leq \frac{c(x,s_1)}{|B(x,s_1^{1/2})|} \frac{c(y,s_2)}{|B(y,s_2^{1/2})|} \langle e^{L(t+s_1+s_2)} \chi_{B(x,s_1^{1/2})}, \chi_{B(y,s_2^{1/2})} \rangle.$$

The proof is completed by applying Theorem 2. □

Example 4 If M is a complete Riemannian manifold with non-negative Ricci curvature, and we put $\sigma = 1$, then it follows from [19] (see also [8, p. 163]) that

$$u(x,t) \le u(y,t+s)\left(\frac{t+s}{t}\right)^{N/2} \exp\left[\frac{d(x,y)^2}{4s}\right].$$

It follows that we may take

$$c(x,s) = 2^{N/2}e^{1/4} \equiv c$$

in (H1). Putting $s_1 = s_2 = s$, Theorem 3 now yields

$$0 \le K(t,x,y) \le c^2|B(x,s^{1/2})|^{-1/2}|B(y,s^{1/2})|^{-1/2}\exp\left\{-\frac{(d(x,y)-2s^{1/2})_+^2}{4(t+2s)}\right\}$$

provided $0 < s < t$. The Li–Yau upper bound on K, [19], [8, p. 170], follows from this upon putting $s = \varepsilon t$ where $0 < \varepsilon < 1$.

An entirely similar calculation may be carried out if the Ricci curvature is bounded below by a negative constant [7, 8, 19].

The statement and proof of Theorem 3 are still valid if one replaces (H1) by the following hypothesis:

(H2) There exists a constant $c(x,s)$ such that

$$0 \le u(x,s) \le c(x,s)u(y,2s)$$

whenever $y \in B(x,s^{1/2})$ and u is a positive solution of

$$\frac{\partial u}{\partial t} = \sigma^{-2}\nabla\cdot(\sigma^2\nabla u)$$

on $B(x,2s^{1/2}) \times (0,2s]$.

Since we are using what is usually considered to be a deeper property, the parabolic Harnack inequality, to prove a more superficial pointwise Gaussian upper bound, some comments are needed. Firstly we emphasize that we have the constant 4 inside the exponential of the Gaussian upper bound even though we make no global assumptions about M, σ or Δ. The parabolic Harnack inequality is only needed in a neighbourhood of x and y in order to get an upper bound on $K(t,x,y)$. If $\sigma = 1$ and one has local lower bounds on the Ricci tensor around x, then suitable constants $c(x,s)$ can be obtained for small s from [19, Theorem 2.1]. There are several other methods of obtaining suitable constants $c(x,s)$ for small s based upon the use of a local coordinate system around x [6, 9, 22]. If we do not assume that the metric is smooth, geodesics may not be definable as solutions of a first order differential equation on M, the exponential map may not exist, and we cannot use normal coordinates in small neighbourhoods. This accounts for the slightly cumbersome form of the following hypothesis:

(H3) We say that M, σ has weak bounded geometry if there are positive constants c_1 and r and a diffeomorphism

$$\Phi_x : \{y : \|y\| < r\} \subseteq \mathcal{R}^N \to U_x \subseteq M$$

for all $x \in M$, with $\Phi_x(0) = x$ and the following properties. If $y \in U_x$ then

$$c_1^{-1} \le \frac{\sigma(y)}{\sigma(x)} \le c_1.$$

Considering $\{y : \|y\| < r\}$ as a coordinate patch, the metric satisfies

$$c_1^{-1} \le g_{ij}(y) \le c_1.$$

Under the above conditions if we define the distorted balls $\tilde{B}(x, \rho)$ for $0 < \rho < r$ by

$$\tilde{B}(x, \rho) = \Phi_x\{y : \|y\| < \rho\}$$

then there exists a constant $c_2 = c_2(c_1, N)$ such that

$$c_2^{-1}\sigma(x)^2\rho^N \le |\tilde{B}(x, \rho)| \le c_2\sigma(x)^2\rho^N$$

and $z \in \tilde{B}(x, \rho)$ implies $d(x, z) \le c_2\rho$.

By Moser's parabolic Harnack inequality [9, 22] we have the following further crucial information.

Lemma 5 *There is a positive constant $c_3 = c_3(c_1, N)$ such that if $0 < 2s^{1/2} < r$ and u is a positive solution of*

$$\frac{\partial u}{\partial t} = \sigma^{-2}\nabla \cdot (\sigma^2 \nabla u)$$

on $\tilde{B}(x, 2s^{1/2}) \times (0, 2s)$ then

$$0 \le u(x, s) \le c_3 u(y, 2s)$$

for all $y \in \tilde{B}(x, s^{1/2})$. *In particular*

$$0 \le u(x,s) \le \frac{c_3}{|\tilde{B}(x,s^{1/2})|} \int_{\tilde{B}(x,s^{1/2})} u(y,2s)\sigma(y)^2 d\,\mathrm{vol}(y).$$

An alternative proof of the following theorem may be obtained by first treating only the case $x = y$, which is the simplest one, and then using the much deeper methods of [7, 8, 10]. We prefer to give a completely self-contained treatment.

Theorem 6 *Suppose that* M, σ *has weak bounded geometry in the sense of* (H3). *Then*

$$0 \le K(t,x,y) \le c_4 \sigma(x)^{-1}\sigma(y)^{-1} \max\left\{ \left(\frac{2}{r}\right)^N, t^{-N/2}, \left(\frac{d}{t}\right)^N \right\} e^{-d^2/4t}$$

for all $x, y \in M$ *and* $t > 0$, *where* $d = d(x,y)$ *and* $c_4 = c_4(c_1, N)$.

Proof We first combine the method of proof of Theorem 3 and Lemma 5, but with $\tilde{B}(x, s^{1/2})$ replacing $B(x, s^{1/2})$. This yields

$$(2.1) \qquad 0 \le K(t,x,y) \le c_5 \sigma(x)^{-1}\sigma(y)^{-1} s^{-N/2} \exp\left[- \frac{(d(x,y) - 2c_2 s^{1/2})_+^2}{4(t+2s)} \right]$$

provided $0 < s \le \min(t, r^2/4)$. We treat three cases separately.

Case 1. If $d^2 \le t$ we put $s = \min(t, r^2/4)$ so that

$$\begin{aligned} s^{-N/2} &= \max\left\{ \left(\frac{2}{r}\right)^N, t^{-N/2} \right\} \\ &= \max\left\{ \left(\frac{2}{r}\right)^N, t^{-N/2}, \left(\frac{d}{t}\right)^N \right\}. \end{aligned}$$

We now use (2.1) to obtain

$$\begin{aligned} 0 \le K(t,x,y) &\le c_5 \sigma(x)^{-1}\sigma(y)^{-1} \max\left\{ \left(\frac{2}{r}\right)^N, t^{-N/2}, \left(\frac{d}{t}\right)^N \right\} \\ &\le c_6 \sigma(x)^{-1}\sigma(y)^{-1} \max\{\cdots\} e^{-d^2/4t}. \end{aligned}$$

Case 2. If $d^2 > t$ and $t/d > r/2$ we put

$$s = \frac{r^2}{64 c_2^2} \le \frac{r^2}{4}.$$

We also have

$$s \leq \frac{1}{16c_2^2}\frac{t^2}{d^2} \leq \frac{1}{16c_2^2}t \leq t$$

so s is a permissible value. Now

$$d - 2c_2 s^{1/2} = d - 2c_2\frac{r}{8c_2} = d - \frac{r}{4} \geq 0$$

so

$$(d - 2c_2 s^{1/2})_+^2 = \left(d - \frac{r}{4}\right)^2 \geq d^2 - \frac{dr}{2} \geq d^2 - t > 0.$$

Since

$$\frac{r^2}{32c_2^2 t} < \frac{1}{8c_2^2 t}\frac{t^2}{d^2} \leq \frac{t}{d^2} < 1$$

we have

$$\begin{aligned}(t+2s)^{-1} &= t^{-1}\left(1 + \frac{r^2}{32c_2^2 t}\right)^{-1} \\ &\geq t^{-1}\left(1 + \frac{t}{d^2}\right)^{-1} \\ &\geq t^{-1}\left(1 - \frac{t}{d^2}\right) > 0.\end{aligned}$$

Therefore

$$\begin{aligned}\frac{(d - 2c_2 s^{1/2})_+^2}{4(t+2s)} &\geq \frac{d^2 - t}{4t}\left(1 - \frac{t}{d^2}\right) \\ &= \frac{d^2}{4t}\left(1 - \frac{t}{d^2}\right)^2 \\ &\geq \frac{d^2}{4t}\left(1 - 2\frac{t}{d^2}\right) \\ &\geq \frac{d^2}{4t} - 1.\end{aligned}$$

Also

$$s^{-N/2} = c_7\left(\frac{2}{r}\right)^N = c_7 \max\left\{\left(\frac{2}{r}\right)^N, t^{-N/2}, \left(\frac{d}{t}\right)^N\right\}$$

so (2.1) yields

$$\begin{aligned}0 \leq K(t,x,y) &\leq c_5 c_7 \sigma(x)^{-1}\sigma(y)^{-1}\max\{\cdots\}\exp\left\{-\frac{d^2}{4t} + 1\right\} \\ &= c_8 \sigma(x)^{-1}\sigma(y)^{-1}\max\{\cdots\}\exp\left\{-\frac{d^2}{4t}\right\}.\end{aligned}$$

Case 3. If $d^2 > t$ and $t/d \le r/2$ we put

$$s = \frac{t^2}{16c_2^2 d^2} \le \frac{t^2}{d^2} \le \min\left\{t, \frac{r^2}{4}\right\}$$

so s is a permissible value. We have

$$\begin{aligned}(t+2s)^{-1} &= t^{-1}\left(t + \frac{t}{8c_2^2 d^2}\right)^{-1} \\ &\ge t^{-1}\left(1 + \frac{t}{d^2}\right)^{-1} \\ &\ge t^{-1}\left(1 - \frac{t}{d^2}\right) > 0.\end{aligned}$$

Also

$$\begin{aligned}d - 2c_2 s^{1/2} &= d - 2c_2 \frac{t}{4c_2 d} \\ &= d\left(1 - \frac{t}{2d^2}\right) > 0\end{aligned}$$

so

$$(d - 2c_2 s^{1/2})_+^2 \ge d^2\left(1 - \frac{t}{2d^2}\right)^2 \ge d^2\left(1 - \frac{t}{d^2}\right) > 0.$$

Therefore

$$\begin{aligned}\frac{(d - 2c_2 s^{1/2})_+^2}{4(t+2s)} &\ge \frac{d^2}{4t}\left(1 - \frac{t}{d^2}\right)^2 \\ &\ge \frac{d^2}{4t}\left(1 - \frac{2t}{d^2}\right) \ge \frac{d^2}{4t} - 1.\end{aligned}$$

Now

$$s^{-N/2} = c_9\left(\frac{d}{t}\right)^N = c_9 \max\left\{\left(\frac{2}{r}\right)^N, t^{-N/2}, \left(\frac{d}{t}\right)^N\right\}$$

so (2.1) yields

$$\begin{aligned}0 &\le K(t,x,y) \le c_5 c_9 \sigma(x)^{-1}\sigma(y)^{-1} \max\{\cdots\} \exp\left\{-\frac{d^2}{4t} + 1\right\} \\ &= c_{10}\sigma(x)^{-1}\sigma(y)^{-1} \max\{\cdots\} \exp\left\{-\frac{d^2}{4t}\right\}.\end{aligned}$$

□

3. Conservation of probability and the Feller property

In this section we use the previous results to prove the above-named properties under hypotheses which do not mention pointwise curvature bounds. Apart from allowing a general weight σ, our proof of conservation of probability is similar to that of [2, 13, 18], and we include it mainly for completeness. We believe, however, that our theorem on the Feller property is new. Applications of these theorems may be found in [13, 20, 25, 26] and in the next section.

Theorem 7 *If M is a complete Riemannian manifold and*

$$|B(p,r)| \leq a\exp(br^2)$$

for some $p \in M$, $a, b, > 0$ and all $r > 0$, then the semigroup e^{Lt} on $L^1(M, \sigma^2 dx)$ is conservative.

Proof If $f \geq 0$ has bounded support we put

$$\psi(x) = \mathrm{dist}(x, \mathrm{supp} f).$$

We also put $\phi = e^{\alpha\psi}$ where $\alpha = m/2t$. If m is large enough then $m-1 < d(x,p) \leq m$ implies $\psi(x) \geq m - c$, where $c > 0$ depends upon p and the support of f. Next put

$$g_m(x) = \begin{cases} 1 & \text{if } d(x,p) \leq m-1, \\ m - d(x,p) & \text{if } m-1 < d(x,p) \leq m, \\ 0 & \text{if } d(x,p) > m, \end{cases}$$

and put

$$S_m = \{x : m-1 < d(x,p) \leq m\}.$$

Then $u_t = e^{Lt}f$ satisfies

$$\begin{aligned}
\langle f, g_m\rangle - \langle u_t, g_m\rangle &= -\int_0^t \frac{d}{ds}\langle u_s, g_m\rangle ds \\
&= \int_0^t \langle \bar{\nabla} u_s, \nabla g_m\rangle ds \\
&= \int_0^t \langle \phi\bar{\nabla} u_s, \phi^{-1}\nabla g_m\rangle ds \\
&\leq \left[\int_0^t \|\phi\bar{\nabla} u_s\|_2^2 ds \int_0^t \|\phi^{-1}\nabla g_m\|_2^2 ds\right]^{1/2} \\
&\leq [2e^{2\alpha^2 t}\|f\phi\|_2^2 e^{-2\alpha(m-c)} t|S(m)|]^{1/2} \\
&\leq [2\|f\|_2^2 ta\exp(2\alpha^2 t - 2\alpha(m-c) + bm^2)]^{1/2} \\
&\leq \left[2\|f\|_2^2 ta\exp\left(\frac{m^2}{2t} - \frac{m(m-c)}{t} + bm^2\right)\right]^{1/2}
\end{aligned}$$

This converges to zero as $m \to \infty$ provided $0 < t < (2b)^{-1}$. We conclude that

$$\langle f, 1\rangle \leq \langle u_t, 1\rangle$$

for all $f \geq 0$ of bounded support and all $0 < t < (2b)^{-1}$. This implies the conservation of probability for all $0 < t < (2b)^{-1}$ by standard density arguments, and the result for all $t > 0$ then follows by an application of the semigroup property. □

We next turn to the Feller property. Since $e^{Lt} : L^\infty \to L^\infty$ is bounded, one has $e^{Lt}(C_0) \subseteq C_0$ if $e^{Lt}(C_c) \subseteq C_0$ where C_c is the space of continuous functions of compact support. Since

$$e^{Lt}f(x) = \int_B K(t, x, y)f(y)\sigma^2(y)dy$$

where B is the compact support of $f \in C_c$, we find that the problem is to prove that

$$\lim_{x\to\infty} K(t, x, y) = 0$$

for all $y \in M$ and $t > 0$. Indeed using the semigroup property it is sufficient to do this for $0 < t < T$, where T is arbitrarily small (independently of y). Another version of the following theorem was obtained independently by Pang [25].

We suppose that $c > 0$ and that for each $x \in M$ there exists $r(x) > 0$, called the bounded geometry radius at x, with the following property. The ball $B(x, r(x))$ can be mapped diffeomorphically onto the coordinate patch U in $\mathcal{R}^N$ given by

$$U = \{y \in \mathcal{R}^N : \|y\| < r(x)\}$$

in such a way that for any $y, z \in U$ one has

$$c^{-1} \le g_{ij}(z) \le c,$$

$$c^{-1} \le \sigma(y)/\sigma(z) \le c.$$

If $\sigma(x)$ and the metric depend continuously upon $x \in M$, then such an $r(x) > 0$ always exists and one should take it as large as possible, but in the general case the existence of $c > 0$ for which such an $r(x) > 0$ exists is a hypothesis.

In the case $\sigma = 1$, the condition of the theorem below on the rate at which the bounded geometry radius $r(x)$ can vanish as $x \to \infty$ may be related to stronger conditions [5, 18] about the rate at which the sectional curvature can tend to minus infinity as $x \to \infty$.

Theorem 8 *Let M be a complete Riemannian manifold. If there exist $p \in M$ and positive constants c_1, c_2 such that the bounded geometry radius $r(x)$ satisfies*

$$\sigma(x)^2 \min\{r(x), 1\}^N \ge c_1 \exp[-c_2 d(x, p)^2]$$

for all $x \in M$, then e^{Lt} has the Feller property.

Proof Assuming that $0 < t \le \frac{1}{4}$ we put

$$s(x) = t \min\{r(x), 1\}^2$$

so that $0 < s(x) \le t$ and $0 < 2s(x) \le r(x)$.

The ellipticity constants of L in $B(x, 2s(x)^{1/2})$ are bounded independently of x. So the parabolic Harnack inequality [9, 22] yields

$$c(x, s(x)) \le c_3$$

for all $x \in M$. The uniform geometry in $B(x, r(x))$ also implies that

$$c_4^{-1} \sigma(x)^2 s(x)^{N/2} \le |B(x, s(x)^{1/2})| \le c_4 \sigma(x)^2 s(x)^{N/2}$$

for all $x \in M$. Applying Theorem 3 under the hypothesis (H2) instead of (H1) we obtain

$$\begin{aligned}
0 &\leq K(t,x,y) \\
&\leq c_3^2 c_4 \sigma(x)^{-1} s(x)^{-N/4} \sigma(y)^{-1} s(y)^{-N/4} \exp\left[-\frac{(d(x,y)-s(x)^{1/2}-s(y)^{1/2})_+^2}{4(t+s(x)+s(y))}\right] \\
&\leq c_3^2 c_4 t^{-N/2} \sigma(x)^{-1} \min\{r(x),1\}^{-N/2} \sigma(y)^{-1} \min\{r(y),1\}^{-N/2} \\
&\quad \times \exp\left[-\frac{(d(x,y)-2t^{1/2})_+^2}{12t}\right] \\
&\leq c_5(y) t^{-N/2} \exp\left[\frac{c_2}{2} d(x,p)^2 - \frac{(d(x,y)-2t^{1/2})_+^2}{12t}\right].
\end{aligned}$$

If $6c_2 t < 1$, then this converges to zero as $x \to \infty$ for all y. □

4. Applications of the theory

In this section we show that the theory we have described yields results concerning a variety of singular elliptic operators and singular Schrödinger operators on Euclidean space.

We put $M = \mathcal{R}^N$ and let H be the non-negative self-adjoint operator on $L^2(\mathcal{R}^N, A dx)$ associated with the quadratic form

$$Q(f) = \int_{\mathcal{R}^N} \Sigma D_{ij}(x) \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} d^N x \tag{4.1}$$

so that formally one has

$$Hf = -A^{-1} \sum \frac{\partial}{\partial x_i}\left(D_{ij} \frac{\partial f}{\partial x_j}\right).$$

We assume that $A(x)^{\pm 1}$ are measurable and locally bounded on $\mathcal{R}^N$. We assume that $D_{ij}(x)$ is a real symmetric matrix which has bounded distortion in the sense that

$$D_{ij}(x) = B(x) C_{ij}(x)$$

where $\det C(x) = 1$ and

$$0 < c^{-1} \leq C(x) \leq c < \infty$$

for all $x \in \mathcal{R}^N$. We also assume that $B(x)^{\pm 1}$ are locally bounded. We then have

$$c^{-1} Q'(f) \leq Q(f) \leq c Q'(f)$$

where

$$Q'(f) = \int_{\mathcal{R}^N} B|\nabla f|^2 d^N x.$$

We now put

$$\rho = B^{-1}A, \quad \sigma = B^{N/4}A^{1/2-N/4}$$

or equivalently

$$B = \sigma^2 \rho^{N/2-1}, \quad A = \sigma^2 \rho^{N/2}$$

to obtain

$$Q(f) = \int \sum C_{ij} \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} \sigma^2 \rho^{N/2-1} d^N x \tag{4.2}$$

and

$$\|f\|_2^2 = \int |f|^2 \sigma^2 \rho^{N/2} d^N x. \tag{4.3}$$

If we introduce the Riemannian metric

$$ds^2 = \sum \rho(x) \{C(x)^{-1}\}_{ij} dx_i dx_j \tag{4.4}$$

then it has volume element

$$d \text{ vol} = \rho^{N/2} d^N x$$

and is quasiconformal in the sense that

$$c^{-1}\rho(x)dx^2 \leq ds^2 \leq c\rho(x)dx^2$$

for all $x \in \mathcal{R}^N$. We can then rewrite (4.1) or (4.2) in the form

$$Q(f) = \int |\nabla f|^2 \sigma^2 d \text{ vol}$$

and (4.3) in the form

$$\|f\|_2^2 = \int |f|^2 \sigma^2 d \text{ vol}.$$

This enables us to identify H with $-L$.

Lemma 9 *If*

$$B^{-1}(x)A(x) \geq c_1(1+x^2)^{-1}$$

for some $c_1 > 0$ and all $x \in \mathcal{R}^N$, then $\mathcal{R}^N$ is complete for the metric (4.4). If

$$B^{-1}(x)A(x) \geq c_1(1+x^2)^{\alpha-1}$$

for some $c_1 > 0, \alpha > 0$ *and all* $x \in \mathcal{R}^N$ *then*

$$d(x,0) \geq c_2|x|^\alpha$$

for some $c_2 > 0$ *and all large enough* $|x|$.

Proof In the first case we have

$$ds \geq c_3(1+x^2)^{-1/2}|dx|$$

so

$$\begin{aligned} d(x,0) &\geq \int_0^{|x|} c_3(1+r^2)^{-1/2}dr \\ &\sim \log|x| \end{aligned}$$

as $|x| \to \infty$. Since log diverges this implies completeness. In second case

$$\begin{aligned} d(x,0) &\geq \int_0^{|x|} c_4(1+r^2)^{(\alpha-1)/2}dr \\ &\sim |x|^\alpha \end{aligned}$$

as $|x| \to \infty$.

The following theorem introduces the function

$$\bar{A}(r) = \int_{S^{N-1}} A(r\omega)dS(\omega).$$

□

Theorem 10 *If*

$$A(x)/B(x) \geq c_5|x|^{2\alpha-2}$$

for large enough $|x|$, *where* $c_5 > 0$ *and* $\alpha > 0$ *and*

$$\bar{A}(r) \leq \delta \exp(\gamma r^\beta)$$

for all $r > 0$, *where* β, γ, δ *are positive constants and* $\beta \leq 2\alpha$, *then the semigroup* e^{Lt} *on* $L^1(\mathcal{R}^N, Adx)$ *conserves probability.*

Proof For large enough r we have

$$\begin{aligned}|B(0,r)| &= \int\limits_{d(0,x)\le r} A(x)dx \\ &\le \int\limits_{|x|\le c_6 r^{1/\alpha}} A(x)dx \\ &\le \int_0^{c_6 r^{1/\alpha}} \delta \exp(\delta s^\beta) c_N s^{N-1} ds \\ &\le c_7 \exp(\gamma' r^{\beta/\alpha}).\end{aligned}$$

One may now apply Theorem 7. □

We now specialize even further to the case where $M = \mathcal{R}^N$, $\sigma^{\pm 1} \in L^\infty_{\text{loc}}$,

$$Q(f) = \int\limits_{\mathcal{R}^N} |\nabla f|^2 \sigma^2 d^N x, \tag{4.5}$$

$$\|f\|_2^2 = \int\limits_{\mathcal{R}^N} |f|^2 \sigma^2 d^N x, \tag{4.6}$$

so that the metric (4.4) is the Euclidean metric.

The operator H on $L^2(\mathcal{R}^n, \sigma^2 d^N x)$ associated with Q is unitarily equivalent to $H' = UHU^{-1}$ on $L^2(\mathcal{R}^n, d^N x)$ where the unitary operator U from $L^2(\mathcal{R}^n, \sigma^2 d^N x)$ to $L^2(\mathcal{R}^n, d^N x)$ is defined by $Uf = \sigma f$. We call H' a "singular Schrödinger operator" since it is of the form

$$H'f = -\Delta f + Vf$$

with $V = \Delta\sigma/\sigma$, provided σ is sufficiently smooth. In [8, §4.7] we used the theory of Schrödinger operators to investigate H, but it is now possible to argue in the reverse direction! Note that σ may be the ground state eigenfunction of H', but we need not assume that $\sigma \in L^2(\mathcal{R}^N, d^N x)$.

The hypothesis on σ in the next theorem corresponds in some sense to the "potential" V being uniformly bounded "on average" in $\mathcal{R}^N$.

Theorem 11 *Suppose that there are positive constants c_1 and r such that the positive weight σ on $\mathcal{R}^N$ satisfies*

$$c_1^{-1} \le \frac{\sigma(x)}{\sigma(y)} \le c_1$$

whenever $|x-y| \leq r$. *Then the heat kernel* K' *of the "singular Schrödinger operator"* H' *satisfies*

$$0 \leq K'(t,x,y) \leq c_4 \max\left\{\left(\frac{2}{r}\right)^N, t^{-N/2}, \frac{|x-y|^N}{t^N}\right\} \exp\left[-\frac{|x-y|^2}{4t}\right]$$

for all $t > 0$ *and* $x, y \in \mathcal{R}^N$, *where* $c_4 = c_4(c_1, N)$.

Proof This follows from Theorem 6, once one observes that

$$K'(t,x,y) = \sigma(x)\sigma(y)K(t,x,y).$$

□

Note. One cannot expect to improve this bound for large t when $x = y$, since 0 may be an eigenvalue of H'.

We now study the Feller property for (4.5) and (4.6) but for a different class of weights.

Theorem 12 *Suppose that there is a constant* $c \geq 1$ *such that*

$$\sigma(x) \geq c^{-1}e^{-cx^2}$$

for all $x \in \mathcal{R}^N$, *and*

$$c^{-1} \leq \frac{\sigma(x)}{\sigma(y)} \leq c$$

for all $x, y \in \mathcal{R}^N$ *such that*

$$|x-y| \leq c^{-1}(1+|x|)^{-c}.$$

Then the semigroup e^{-Ht} *on* $L^2(\mathcal{R}^N, \sigma^2 dx)$ *associated with (4.5) and (4.6) has the Feller property.*

Note. This theorem may be compared with Theorem 4.7.3 of [8], which assumes that the "Schrödinger operator" H' has a genuine potential which is bounded below.

Proof This is an application of Theorem 8 with $p = 0$ and

$$r(x) = c^{-1}(1+|x|)^{-c}.$$

□

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